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MULTICOMPONENT VLE CALCULATIONS
BY UNIQUAC AND UNIFAC

by

ALİ AYLA

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MULTICOMPONENT VLE CALCULATIONS
BY UNIQUAC AND UNIFAC

APPROVED BY :

Prof.Dr.Salih DİNÇER Salih Dinçer
(Thesis Supervisor)

Yrd.Doç.Dr.İvet BAHAR Bahar

Yrd.Doç.Dr.İbrahim YILMAZ

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ABSTRACT

Vapor-liquid equilibrium data is essential and fundamental for design of separation equipment. If available, experimental data are of course the best, but when such data are not available, the engineer has to apply thermodynamic relations to phase equilibrium calculations.

In this study, since the equations for phase equilibria are complex and require trial and error methods, a computer program was prepared for this purpose. The program uses UNIQUAC and UNIFAC equations for liquid phase nonideality and Peng-Robinson equation for vapor phase nonideality. The program can also perform calculation for systems containing noncondensable components at infinite dilution. Totally 1500 data points of thirty-three binary systems and four ternary systems were studied. The results calculated using UNIQUAC and UNIFAC equations were compared against experimental results. For comparison purposes, the systems were also simulated using Raoult's law.

As a result, it is observed that UNIQUAC and UNIFAC equations are in good agreement with experimental data, mostly

much better than those by Raoult's law. Also, it can be seen that Peng-Robinson equation gives good results for vapor phase nonideality. Unfortunately, the results for condensable-noncondensable systems were not encouraging.

ÖZET

Buhar-sıvı denge verileri ayırma işlemlerinin tasarımında temel ve önemli bir yer tutmaktadır. Deneysel veriler her zaman tercih edilmesine rağmen, bunların eksikliğinde, mühendis faz dengesi hesaplamaları için termodinamik bağıntıları kullanmak zorundadır.

Bu çalışmada, faz dengesi hesaplamaların karışıklığı ve deneme-yanılma yöntemlerine gereksinim duyulması nedeniyle, bir bilgisayar programı hazırlanmıştır. Bu program sıvı faz için UNIQUAC ve UNIFAC eşitliklerini, buhar fazı içinde Peng-Robinson hal denklemini kullanmaktadır. Program kritik üstü yoğuşmayan maddeler içeren sistemlerin de faz dengesi hesaplamalarını yapabilmektedir. Bu çalışmada outzüç ikili ve dört adet üçlü sistem yaklaşık 1500 denge noktası için incelenmiştir. UNIFAC ve UNIQUAC eşitliklerinden alınan sonuçlar hem deneysel verilerle hem de kendi aralarında karşılaştırılmıştır. Yine karşılaştırma amacı ile sonuçlar bir kez de Raoult yasası kullanılarak elde edilmiştir.

Sonuç olarak, UNIQUAC ve UNIFAC eşitliklerinin genelde deneysel değerlerle iyi uyum sağladığı ve bu sonuçların

Raoult yasası ile alınan sonuçlardan çok daha iyi olduğu gözlenmiştir. Buhar fazın ideallikten sapma durumu için, Peng-Robinson denkleminin çalışılan sistemlerde iyi sonuç verdiği görülmüştür. Fakat kritik üstü maddeler içeren sistemler için alınan sonuçlar, yoğuşabilir sistemler için alınan sonuçlar kadar tatmin edici olmamıştır.

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A,B,C	Constants of Antoine Equation
a	A constant defined by Eq.(2.27)
a_{ij}	UNIQUAC or UNIFAC energy parameters.
b	A constant defined by Eq.(2.28)
F	The degrees of freedom in phase rule
$\hat{f}_i$	Fugacity of component i in solution.
f_i^o	Standart state fugacity of pure component i
G^E	Excess Gibbs free energy
H_i	Henry's constant of solute i.
K	Equilibrium ratio (y/x)
l_i	A constant defined by Eq.2.61
m	Number of phases
N	Number of components
P	Pressure
q_k	Surface parameter in combinatorial part of UNIQUAC.
q_k'	Surface parameter in residual part of UNIQUAC.
Q_k	Group area parameter in UNIFAC
r_k	Volume parameter in UNIQUAC.

R_k	Group volume parameter in UNIFAC.
R	Universal gas constant.
T	Temperature
T_r	Reduced Temperature
U_{ij}	Energy interaction between groups i and j in UNIFAC.
V	Vapor molar volume
$\bar{v}_i^L$	Partial liquid molar volume.
v_i^L	Liquid molar volume
x	Liquid phase mole fraction
y	Vapor phase mole fraction
z	Compressibility factor.
Z_a	Rackett parameter
z	Coordination number in UNIQUAC and UNIFAC
γ_i	Activity coefficient of component i
ε	A parameter in Eq. (A.1.1)
θ_i	Area fraction of component i in combinatorial part of activity coefficient
θ_i'	Area fraction of component i in residual part of activity coefficient
μ_i	Chemical potential of component i in solution
τ_{ij}	Interaction parameter in UNIQUAC

δ_{ij}	Interaction parameter in Peng-Robinson Equation.
$\delta_{ij}^{(o)}, \delta_{ij}^{(1)}$	Parameter for solute i in solventj.
Ψ_{mn}	Interaction parameter in UNIFAC.
Φ	Segment fraction
ϕ	Fugacity coefficient
$\hat{\phi}_i$	Fugacity coefficient of component i in solution.
α	Scaling factor in Peng-Robinson Equation
ω	Acentric factor

Subscripts

i,j,k	Components i,j, and k in a solution
ij	Characteristic property used for i-j binary
c	Critical property

Superscript

L	Liquid phase
m	m'th phase
s	Saturation conditions
V	Vapor phase

I. INTRODUCTION

Separation of fluid mixtures constitutes one of the main tasks of chemical engineering. Most large scale separations are achieved by classical phase contacting operations : distillation, absorption, stripping and extraction. Design of equipment for such operations requires favorable relationships between the equilibrium states of two or more phases for their success.

The possible number of liquid and vapor mixtures in technological processes is incredibly large, and it is unreasonable to expect the experimental vapor-liquid equilibria will ever be available for a significant fraction of this number. Further, obtaining good experimental data requires appreciable experimental skill,experience,and patience. It is, therefore, an economic necessity to consider techniques for calculating phase equilibria.

Multicomponent vapor-liquid equilibrium calculations require iterative schemes on account of the complex composition functionality implicit in the equations which describe the equilibrium. Instead of approximate solutions based on a variety of simplifying assumptions, solutions well which the accuracy of the data may be obtained by use of computer.

This study presents a computer program(VLENC) for the estimation of vapor-liquid equilibria by using UNIQUAC and UNIFAC. The results are discussed by giving various examples.

2. THERMODYNAMICS OF EQUILIBRIUM

The thermodynamic treatment of multicomponent phase equilibria is based on the concept of chemical potential.Two or more phases being in thermodynamic equilibrium means that the temperature of each phase is the same and the chemical potential of each component present is equal to its chemical potential in other phases :

$$T^1 = T^2 = \dots\dots\dots T^m \tag{2.1a}$$

$$\mu_i^1 = \mu_i^2 = \dots\dots\dots \mu_i^m \tag{2.1b}$$

where T, μ, and m stand for temperature, chemical potential and the number of phases, respectively. But, for engineering purposes, a physically more meaningful quantity, called fugacity, can be obtained by a simple transformation. Fugacity can be considered as a thermodynamic pressure since the fugacity of each component is equal to its partial pressure in a mixture of ideal gases.

For vapor-liquid equilibria, at the same temperature, the equation of equilibrium for each component i is expressed in terms of fugacity $\hat{f}i$:

$$\hat{f}_i^V = \hat{f}_i^L \qquad (2.2)$$

where v and L stand for vapor and liquid phases, respectively.

In order to be able to use Eq.(2.2), the fugacities should be related to the experimentally accessible quantites such as liquid mole fraction x, vapor mole fraction y, absolute temperature T and total pressure P. In thermal and mechanical equilibrium, temperature and pressure are assumed to be same for both phases. Fugacities can be related to these accessible quantities using two auxiliary functions which are called fugacity coefficient ϕ and activity coefficient γ . Fugacity coefficient of a component i in amixture ($\hat{\phi}_i$) is defined by:

$$\hat{\phi}_i = \frac{\hat{f}_i^V}{y_i P} \qquad (2.3)$$

where superscript v stands for vapor phase. Activity coefficient can be expressed as :

$$\gamma_i = \frac{\hat{f}_i^V}{x_i \; f_i^{oL}} \qquad (2.4)$$

where f_i^{oL} is the standart state fugacity of component i and superscript L stands for liquid phase. Substituting Eqs.(2.3) and (2.4) in Eq. (2.2) yields :

$$\hat{\phi}_i \, y_i P = \gamma_i \, x_i \, f_i^{oL} \qquad (2.5)$$

This equation is the key equation in the calculation of multicomponent vapor-liquid equilibria.

2.1. Symmetric and Unsymmetric Conventions for Normalization

As indicated in Eq(2.4), the activity coefficient can not be defined unless the standart-state fugacity f_i^{oL} , is clearly specified. It is convenient to think that standart state fugacity f_i^{oL} be the fugacity of component i as a pure liquid at the same temperature of the solution and at some specified pressure. In the choice of standart state fugacity, two different normalizations of activity coefficients for condensable and non-condensable components can be used(1).The normalization of activity coefficient means, specification of the state where in activity coefficient is unity. For condensable compenents, activity coefficient is normalized such that $\gamma_i \longrightarrow 1$ as $x_i \longrightarrow 1$. In that case, the fugacity of a component becomes equal to the mole fraction multiplied by the standart-state fugacity in the limit. For the system, containing only condensable components, it is said that the activity coefficients follow symmetric convention.

However, if the liquid solution contains a noncondensable component, the normalization of activity coefficients applied to condensable components can not be used for noncondensable components, since a pure liquid of supercritical component is physically impossible. Neverthless, the noncondensable components which are not excessively above their critical temperatures can be considered as hypothetical supercritical liquids and their properties can be evaluated by extrapolation. On the other hand, if a noncondensable component is highly above its critical temperature, the concept of hypothetical liquid is of little use since the pure liquid properties obtained by extrapolation in this case lose their physical significance.

Therefore, for a highly supercritical component, it is convenient to use a normalization different from the equation given for condensable components. So, we use $\gamma_i^* \longrightarrow 1$ as $x_i \longrightarrow 0$. The purpose of this asterisk is to call attention to the difference in normalization. According to this different normalization, the fugacity of component i becomes equal to the mole fraction multiplied by the standart-state fugacity of i in the limit as the mole fraction of component i becomes very small. This type of normalization for a noncondensable component yields in the limit an ideal dilute solution or Henry's law region. In that case, the standart-state fugacity of noncondensable component i is defined by Henry's constant.

$$H_i = \lim_{x_i \to 0} \frac{f_i^{oL}}{x_i} \tag{2.6}$$

Since in a multicomponent mixture, containing both noncondensable and condensable components, two different normalizations are applied, in this case, normalization is said to be unsymmetric. In such a mixture, the condensable and noncondensable components are referred to as solvents and solutes, respectively. Briefly, it can be said that, the standart state fugacity of a solvent is the fugacity of a pure liquid and the standart state fugacity of a solute is Henry's constant.

2.2. Standart-State Fugacity for Condensable and Noncondensable Components

The prediction and correlation of physical properties of real materials is greatly facilitated when one has a standart base or a model of "ideal" behaviour to which real behaviour can be compared. For example, a model of ideal behaviour is provided by ideal solutions. In an ideal solution, the fugacity of a component is equal to the mole fraction multiplied with standart state fugacity (2) :

$$f_i^{id} = x_i \, f_i^{oL} \qquad (2.7)$$

Ideal solution is observed in the limiting condition $\gamma_i \longrightarrow 1$ as $x_i \longrightarrow 1$ for condensable component or $\gamma_i^* \longrightarrow 1$ as $x_i \longrightarrow 0$ for a noncondensable component. For the latter case, the standart state fugacity is the Henry's constant.

For a condensable component, the standart state fugacity is given by (3) :

$$f_i^{oL} = P_i^S \phi_i^S \exp \int_{P_i^S}^{P} \frac{V_i^L}{RT} dP \qquad (2.8)$$

where f_i^{oL} = standart-state fugacity at system temperature and pressure P,

P_i^S = saturation vapor pressure of pure liquid at temperature T,

ϕ_i^S = fugacity coefficient of pure saturated vapor, and temperature T,

v_i^L = molar liquid volume of pure i at temperature T.

It is assumed that v_i^L is a function of only temperature, not of pressure.

Normally, Henry's constant for solute 2 in solvent 1 is determined experimentally at the solvent vapor pressure P_1^S. The effect of pressure on Henry's constant is expressed as:

$$H_{2,1}^{(P^r)} = H_{2,1}^{(P_1^S)} \exp \int_{P_1^s}^{P^r} \frac{\overline{V}_2^{\infty}}{RT} dP \qquad (2.9)$$

where ∞ denotes infinite dilution and P^r any reference pressure When P^r is low, the exponential correction in Eq(2.9) is negligible

Since the knowledge of γ_i^* is limited, this study has been concentrated on the mixtures containing dilute solutions of noncondensable components. Therefore, it is convenient to take $\gamma_i^* = 1$ in this study(1). So, for a noncondensable component in dilute region $(X_i \ll 1)$, Eq(2.5) can be re written as:

$$y_i P \hat{\phi}_i = X_i H_{i,j} \qquad (2.10)$$

Subtituting Eq(2.8) into Eq.(2.5), the general equation of vapor-liquid equilibrium for condensable components is written as :

$$y_i P \hat{\phi}_i = X_i \gamma_i P_i^S \phi_i^S \exp \int_{P_1^S}^{P} \frac{V_i^L}{RT} dp \qquad (2.11)$$

2.3 The Vapor Phase Nonideality : Fugacity Coefficient

The vapor-liquid equilibria conditions can be predicted, if the fugacities of two phases are separately calculated.

In the calculation of the fugacities, different techniques are required for vapor and liquid phases.

Vapor phase nonideality becomes important at moderate and high pressure. At low pressures, the gas molecules interact with one another less strongly. Therefore, as total pressure approaches zero, the nonideality of vapor-liquid system mostly exists in the liquid phase. In that case, vapor phase nonideality can be neglected and the fugacity of the vapor phase becomes the product of the vapor mole fraction and total pressure. This is the ideal gas assumption. The less simplified assumption is the Lewis fugacity rule in which the gases are considered as real, but gas solution as ideal(1). For such conditions, the fugacity of component i in a gas solution is the fugacity of pure component i multiplied by its mole fraction. This simplifies calculations because the fugacity coefficient is no longer a function of vapor mole fraction. So, in the prediction of bubble point and flash conditions, no iterations are required for the vapor mole fractions.

Unfortunately, assumption of ideal gas or Lewis fugacity rule, can sometimes cause serious errors, especially at moderate and high pressures. But, with the use of electronic computers, there is no need to make such simplifications

It is often convenient to deal with the ratio of the fugacity to pressure rather than with the fugacity itselt and this ratio is called fugacity coefficient ϕ. There are three such quantities.

For a mixture, $\phi = f/P$ (2.12)

For a pure material, $\phi_i = f_i/P$ (2.13)

For a component in a solution $\hat{\phi}_i = \hat{f}_i/X_iP$ (2.14)

For a mixture or a pure material, fugacity coefficient can be found using the thermodynamic relationship:

$$\ln \phi = \int_0^P (Z-1) \frac{dP}{P} \tag{2.15}$$

where z is the compressibility factor of mixture or pure component. Similar expression is obtained if V, rather than P, is the variable of integration. Then,

$$\ln \phi = (Z-1) - \ln Z - \int_\infty^V (Z-1) \frac{dV}{V} \tag{2.16}$$

The fugacity coefficient of a component i in a solution ($\hat{\phi}_i$) can be expressed as the partial molar property of ln ϕ, where ϕ is the mixture fugacity coefficient :

$$\ln \hat{\phi}_i = \left(\frac{\partial \ln \phi}{\partial X_i}\right)_{T,P,X_{j=i}} \tag{2.17}$$

If the vapor mixture contains only ideal gases, the integral in Eq.(2.15) is zero and Z is unity for all components. In that case ϕ is also unity. In a mixture which contains gases which are not ideal with the gas solution being ideal. the fugacity coefficient of a component i in a solution becomes equal to the fugacity coefficient of a pure component, and then Eq.(2.17) need not be used for vapor phase nonideality.

2.3.1. Peng-Robinson Equation of State

The fugacity coefficient can easily be found from any equation of state. Numerous empirical or semiempirical equations have been proposed up to now. One of them, virial equation of state is the only equation which has a theoretical base. In this study, a new semiempirical equation of state(4), called Peng-Robinson equation of state, is used. Peng-Robinson equation of state is a modified form of vander Waals equation of state.

Semi-empirical equations of state generally express pressure as the sum of two terms, a repulsive pressure P_R and an attactive pressure P_A as follows :

$$P = P_R + P_A \qquad (2.18)$$

The equations of state of vander Waals (1873) and Redlich-Kwong (1949) and Soave (1972) are examples of semiempirical equations and all express the repulsive pressure by the vander Waals hard-sphere equation, similar to Peng-Robinson equation:

$$P_R = \frac{RT}{V-b} \qquad (2.19)$$

The attractive pressure can be expressed as :

$$P_A = - \frac{a}{g(V)} \qquad (2.20)$$

where g(V) is a function of the molar volume and b is constant related to the size of the hard sphere. The parameter a can be regarded as a measure of the intermolecular atractive forces. b is usually treated as temperature indenpendent and a is a constant only in vander Waals equation.

Choosing a suitable function for g(V), the predicted critical compressibility factor can be made to approach a more realistic value. The applicability of the equation at very high pressure is affected by the magnitude of b/V_c, where V_c is the critical volume. Furthermore, treating the dimensionless scaling factor for the energy parameter, as a function of acentric factor in addition to reduced temperature, has significantly improved the prediction of compressibility factor and consequently, the equilibrium ratios (y/x) in mixtures.

In this study. the attractive pressure is calculated from (4) :

$$P_A = - \frac{a(T)}{V(V+b)+b(V-b)} \qquad (2.21)$$

Using Eqs.(2.18),(2,19) and (2.21), one obtains:

$$P = \frac{RT}{V-b} - \frac{a(T)}{V(V+b)+b(V-b)} \qquad (2.22)$$

Eq (2.22) can be rewritten as :

$$Z^3-(1-B)Z^2+(A-3B^2-2B)Z-(AB-B^2-B^3) = 0 \qquad (2.23)$$

where

$$A = \frac{aP}{R^2T^2} \qquad (2.24)$$

$$B = \frac{bP}{RT} \qquad (2.25)$$

$$Z = \frac{PV}{RT} \qquad (2.26)$$

Eq. (2.23) yields one root or three roots depending upon the number of phases in the system. In the two-phase region, the largest root is the compressibility factor of the vapor while the smallest positive root corresponds to that of the liquid.

Using Eq.(2.22), expressions for a and b can be obtained at the critical point :

$$a(T_c) = 0.45724 \frac{R^2 \, T_c{}^2}{P_c} \qquad (2.27)$$

$$b(T_c) = 0.07780 \frac{RT_c}{P_c} \qquad (2.28)$$

$$Z_c = 0.307 \qquad (2.29)$$

At temperatures other than critical :

$$a(T) = (T_c).\,\alpha\ (T_r, \omega) \qquad (2.30)$$

$$b(T) = b(T_c) \qquad (2.31)$$

where $\alpha(T_r, w)$ is a dimensionless function of reduced temperature, T_r, (also called scaling factor for energy) and acentric factor w, and equals unity at the critical temperature. The functional form of α was determined by using the literature vapor pressure values. For all subtances examined, the relationship between α and T_r can be linearized by the following equation :

$$\alpha^{1/2} = 1 + \kappa\ (1 - T_r^{1/2}) \qquad (2.32)$$

where κ is a constant characteristic of each substance. κ values have been correlated against the acentric factor. The resulting equation is :

$$\kappa = 0.37464 + 1.5423\,\omega - 0.26992\,\omega^2 \qquad (2.33)$$

Substituting Eq- (2.22) into Eq.(2.15), an expression for pure component fugacity coefficient is obtained :

$$\ln \phi_i = Z - 1 - \ln(Z - B) - \frac{A}{2\sqrt{2}\,B} \ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right)$$

The fugacity coefficient of component i in a solution can be found by combining Eqs. (2.15),(2.17) and (2.22) :

$$\ln \hat{\phi}_i = \frac{b_i}{b}(Z - 1) - \ln(Z - B)\ \frac{A}{2\sqrt{2}B} \cdot \left(\frac{2\Sigma_k X_k a_{ki}}{a} - \frac{b_i}{b}\right) \ln\left(\frac{Z + 2.414B}{Z - 0.414B}\right)$$

(2.35)

The mixtures parameters used in Eq.(2.35) are defined by the following mixture rules :

$$a = \sum_i \sum_j X_i X_j a_{ij} \qquad (2.36)$$

$$b = \sum_i X_i b_i \qquad (2.37)$$

$$a_{ij} = (1-\delta_{ij})\ a_i^{1/2} a_j^{1/2} \qquad (2.38)$$

In Eq(2.38) δ_{ij} is an empirically determined binary interaction coeffecient, characterizing the i-j binary system. δ_{ij} s are determined using experimental binary VLE data. Its inclusion is necessary in order to bring about better agreement between experimental data and predictions for binary systems involving a hydrocarbon and nonhydrocarbon component. The interaction parameters for several of the water-hydrocarbon binaries are listed in Appendix C, but no interaction parameters is available for hydrocarbon-hydrocarbon binaries (5).

2.4 Liquid Phase Nonideality : Activity Coefficient

In order to predict vapor-liquid equilibria in multicomponent mixtures, we require a method for calculating the fugacity of component i in a liquid phase. First of all, nonideality of the liquid phase has to be expressed. Activity coefficient is used for this purpose. In a mixture, activity coefficient γ_i of component i is related to G^E, the Excess Gibbs free energy per mole of mixture by :

$$G^E = RT \sum_i X_i \ln \gamma_i \qquad (2.39)$$

$$\left(\frac{\partial n_T G^E}{\partial n_i}\right)_{T,P,n_{j=i}} = RT\ln\gamma_i \qquad (2.40)$$

where R is the gas constant, T is the absolute system temperature, n_i is the number of moles of component i, n_T is the total number of moles ($n_T = \sum_i n_i$) and $X_i = h_i/h_T$.

Activity coefficient depends on composition, temperature and pressure. The effect of pressure on activity coefficient is given by :

$$\bar{v}_i^L - v_i^L = RT\left(\frac{\partial \ln\gamma_i}{\partial P}\right)_{T,X_i} \qquad (2.41)$$

where $\bar{v}_i^L$ is partial molar liquid volumes and v_i^L is molar liquid volume. At low or moderate pressures, the effect of pressure is negligible, and in this study, pressure effect on activity coefficient is neglected .

The most important variable is the composition of the component of interest. The effect of temperature is not neglible, but often it is not large when consideration is restricted to a moderate temperature range.

As it is seen in Eq.(2.40),in order to obtain activity coefficients,it is necessary to construct an expression which gives G^E as a function of composition, temperature and pressure. In this study, two different models are used in the calculation of liquid activity coefficients. These models will be discussed in the following sections :

2.4.1 UNIQUAC Equation

A correlation based on the quasi-chemical theory of liquid solutions proposed by Guggenheim(6), and generalized by Abrams and Prausnit2(7), is the UNIQUAC (Universal Quasi Chemical Theory) equation. Unlike Guggenheim's theory, however, UNIQUAC is applicable to mixtures whose molecules differ appreciably in size and shape. One advantage of UNIQUAC is that it contains no more than two adjustable parameters per binary.

UNIQUAC equation, is constructed from a G^E expression which consists of two parts.

$$G^E = G^E\ (\text{combinatorial}) + G^E\ (\text{residual}) \qquad (2.42)$$

for a binary system :

$$\frac{G^E(\text{combinatorial})}{RT} = X_1 \ln\frac{\Phi_1}{X_1} + X_2 \ln\frac{\Phi_2}{X_2} + \left(\frac{Z}{2}\right)\left(q_1 X_1 \ln\frac{\theta_1}{\Phi_1} + q_2 X_2 \ln\frac{\theta_2}{\Phi_2}\right) \qquad (2.43)$$

$$\frac{G^E\text{(residual)}}{RT} = -q_1' X_1 \ln(\theta_1' + \theta_2' \tau_{21}) - q_2' X_2 \ln(\theta_2' + \theta_1' \tau_{12}) \qquad (2.44)$$

where Φ is segment fraction, θ and θ' are area fractions, Z is the coordination number. Z may have a value between 4 and 12 depending on the type of packing. Empirically, for a typical liquid at ordinary conditions, Z is close 10. Numerical results for $\ln \gamma_i$ are insensitive to the choice of Z provided a reasonable value ($6 \leq Z < 12$) is chosen. However, adjustable parameters τ_{ij} and τ_{ji} depend on that choice. In the present work, Z is taken as 10 (8).

Segment fraction Φ and area fractions θ and θ' are given for a binary system by :

$$\Phi_1 = \frac{X_1 r_1}{X_1 r_1 + X_2 r_2} \qquad \Phi_2 = \frac{X_2 r_2}{X_1 r_1 + X_2 r_2} \qquad (2.45)$$

$$\theta_1 = \frac{X_1 q_1}{X_1 q_1 + X_2 q_2} \qquad \theta_2 = \frac{X_2 q_2}{X_1 q_1 + X_2 q_2} \qquad (2.46)$$

$$\theta_1' = \frac{X_1 q_1'}{X_1 q_1 + X_2 q_2} \qquad \theta_2' = \frac{X_2 q_2'}{X_1 q_1 + X_2 q_2} \qquad (2.47)$$

The parameters r, q and q' are pure component molecular structure constants depending on molecular size and external surface areas. r and q are expressed as:

$$r_i = V_{wi}/15.17 \qquad (2.48)$$

$$q_i = A_{wi}/(2.5/10^9) \qquad (2.49)$$

where V_{wi} and A_{wi} are the vander Waals volumes and areas of the molecules given by Bondi(9).

In the original formulation $q=q'$ (7). To obtain better agreement with water or alcohols, q' is used for water and alcohols and they are obtained emprically to give an optimum fit to a variety of systems containing these components(10). For alcohols, the surface, of interaction q', is smaller than the geometric external q, indicating that for alcohols, intermolecular attraction is determined primarily by the-OH groups.

For each bihary combination in a multicomponent mixture, there are two adjustable parameters, τ_{12} and τ_{21}. These in turn are given in terms of characteristic energies Δu_{12} and Δu_{21} by :

$$\tau_{12} = \exp(-\frac{\Delta U_{12}}{RT}) = \exp(-\frac{a_{12}}{T}) \qquad (2.50)$$

$$\tau_{21} = \exp(-\frac{\Delta U_{21}}{RT}) = \exp(-\frac{a_{21}}{T}) \qquad (2.51)$$

Eqs.(2.50) and (2.51) give the primary effect of temperature on τ_{12} and τ_{21} . Charactreristic energies ΔU_{12} and ΔU_{21} are often weakly dependent on temperature. Thus, the atcitivity coefficients are readily found by differentiation as indicated by Eq(2.40).

For a binary mixture, activity coefficient γ_1, is given by :

$$\ln\gamma_1 = \ln\frac{\Phi_1}{X_1} + \left(\frac{Z}{2}\right) q_1 \ln\frac{\theta_1}{\Phi_1} + \Phi_2\left(l_1 - \frac{r_1}{r_2} l_2\right)$$

$$- q'_1 \ln(\theta'_1 + \theta'_2\,\tau_{21}) + \theta'_2 q'_1 \left(\frac{\tau_{21}}{\theta'_2 + \theta'_2\,\tau_{21}} - \frac{\tau_{12}}{\theta'_2 + \theta'_1\,\tau_{12}}\right) \quad (2.52)$$

where $l_1 = \left(\frac{Z}{2}\right)(r_1 - q_1) - (r_1 - 1)$ (2.53)

and $l_2 = \left(\frac{Z}{2}\right)(r_2 - q_2) - (r_2 - 1)$ (2.54)

For component 2, γ_2 can be found by interchanging subscripts 1 and 2.

Eqs.(2.43) and (2.44) can be extended to multicomponent mixtures without additional assumptions as follows :

$$\frac{G^E\text{(combinatorial)}}{RT} = \sum_i X_i \ln\frac{\Phi_i}{X_i} + \frac{Z}{2}\sum_i q_i X_i \ln\frac{\theta_i}{\Phi_i} \quad (2.55)$$

$$\frac{G^E\text{(residual)}}{RT} = -\sum_i q'_i X_i \ln\left(\sum_j \theta'_j\,\tau_{ji}\right) \quad (2.56)$$

where segment fraction Φ and area fractions θ and θ' are given by :

$$\Phi_i = \frac{r_i X_i}{\sum_j r_j X_j} \quad (2.57)$$

$$\theta_i = \frac{q_i X_i}{\sum_j r_j X_j} \tag{2.58}$$

$$\theta'_2 = \frac{q'_i X_i}{\sum_j q'_j X_j} \tag{2.59}$$

For any component i , the activity coefficient can be found by using Eq.(2.40) :

$$\ln\gamma_i = \ln\frac{\Phi_i}{X_i} + \left(\frac{Z}{2}\right) q_i \ln\frac{\theta_i}{\Phi_i} + l_i - \frac{\Phi_i}{X_i}\sum_j X_j l_j - q'_i \ln\left(\sum_j \theta'_j \tau_{ji}\right) + q'_i - q'_i \sum_j \frac{\theta'_j \tau_{ij}}{\sum \theta'_k \tau_{kj}} \tag{2.60}$$

where $l_j = \frac{Z}{2}(r_j - q_j) - (r_j - 1)$ (2.61)

Eq.(2.60) requires only pure component and binary parameters.

In this work, the fugacity of the liquid phase for noncondensable component in dilute region is taken as the mole fraction of that component multiplied by Henry's constant:

$$f_i^L = X_i H_{ij} \tag{2.62}$$

where $H_{i,j}$ shows Henry's constant for solute i in solvent j.

To estimate Henry's constant for solute i in a mixed solvent, the following approximation is used (1):

$$\ln H_{i,M} = \sum_j \theta_j \ln H_{ij} \tag{2.63}$$

where the summation is over all solvents j, and M shows the mixture. The surface fraction θ_j is taken on a solute free basis where solute free refers to all solutes. For convenience, H_{ij}, is expressed as a product of two functions(1):

$$H_{i,j} = (\gamma_{i,j}^{\infty}) \, f_i^{oL} \tag{2.64}$$

where supercript ∞ denotes infinite dilution.

For noncondensable components, the hypothetical standart state fugacity is represented by an arbitrary function(1).

$$\ln \frac{f_i^{oL}}{P_{ci}} = 7.224 - 7.534 \left(\frac{T}{T_{ci}}\right)^{-1} - 2.598 \ln \left(\frac{T}{T_{ci}}\right) \tag{2.65}$$

where P_{ci} and T_{ci} are, respectively, critical pressure and critical temperature of component i. Eq(2.65) gives a rough first approximation for the effect of temperature on Henry's constant. Activity coefficient $\gamma_{i,j}^{\infty}$ is often only weak function of temperature provided that the temperature range is large and provided the system temperature T is not near T_{cj}, the critical temperature of solvent j. Here, $\gamma_{i,j}^{\infty}$ is given by the empirical equation :

$$\ln \gamma_{i,j}^{\infty} = \delta_{i,j}^{(o)} + \delta_{i,j}^{(1)} \, T^{-1} \tag{2.66}$$

where $\delta_{i,j}^{(o)}$ and $\delta_{i,j}^{(1)}$ are binary parameters. For a mixed solvent:

$$\ln\gamma_i^{\infty} = \sum_j \theta_j \ln\gamma_{i,j}^{\infty} \qquad (2.67)$$

where θ_j, again on solute free basis, is the surface fraction of solvent j.

When a condensable solute is present[†], the activity coefficient of a solvent is given by Eq(2.60) provided that all composition variables (X,θ,Φ) are taken on solute free basis. For solutes with small mole fractions, UNIQUAC parameters τ_{ij} and τ_{ji} are set to unity, wherever i is a solute and j is either a solvent or a solute.

UNIQUAC is applicable to nonelectrolyte multicomponent mixtures of nonpolar and polar liquids containing small or large molecules, including polymers, because the primary concentration variable is a surface fraction rather than mole fraction.

2.4.2 UNIFAC Equation

Another model for the prediction of activity coefficients, UNIFAC(UNIQUAC Functional Group Activity Coefficients)(11) is an example of a group contribution method. It is based on the UNIQUAC method. The basic difference is that the liquid mixture is considered to be a solution of structural group is like-CH_3,-OH and others which when added, form the parent

† only volatile gases like H_2,N_2,O_2,CO,Ar and CH_4 are considered to be noncondensable.

molecule. The properties of mixture is then calculated from the properties of the molecules.

Extension of the group-contribution idea to mixtures is extremely attractive because, while the number of pure fluids in chemical technology is already very large, the number of different mixtures is still larger, by many orders of magnitude. Thousands, perhaps millions, of multicomponent liquid mixtures of interest in the chemical industry can be constitued from perhaps at most one hundered functional groups.

In the UNIFAC method, G^E expression and thus activity coefficient has a combinatorial part and a residual part as in UNIQUAC.

$$\ln\gamma_i^c = \ln\gamma_i^c + \ln\gamma_i^R \qquad (2.68)$$

The combinatorial part of the UNIQUAC equation is used directly:

$$\ln\gamma_i^c = \ln\frac{\Phi_i}{X_i} + \frac{Z}{2}\, q_i \ln\frac{\theta_i}{\Phi_i} + l_i - \frac{\Phi_i}{X_i}\sum_j X_j l_j \qquad (2.69)$$

Φ_i, θ_i and l_i are given by Eqs.(2-57),(2-58) and (2-61),respectively z is taken as 10. Only pure component parameters enter into this equation. Parameters r_i and q_i are calculated as the sum of the group volume and area parameters R_k and Q_k :

$$r_i = \sum_k \nu_k^{(i)} R_k \text{ and } q_i = \sum_k \nu_k^{(i)} Q_k \qquad (2.70)$$

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where $\nu_k^{(i)}$ is always an integer, showing the number of groups of type k in molecule i.

Group parameters R_K and Q_k are obtained from the vander Waals group volume and surface areas V_{wk} and A_{wk}, given by Bond (9), as in UNIQUAC equation :

$$R_K = V_{wk}/15.17 \tag{2.71}$$

$$Q_K = A_{wk}/(2.5x10^9) \tag{2.72}$$

The normalization factors 15.17 and $2.5x10^9$ are those given by Abrams and Prausnitz(7).

The residual part of the activity coefficient for the UNIFAC equation is expressed as :

$$\ln\gamma_i^R = \Sigma\nu_k^{(i)} \left| \ln\gamma\Gamma_k - \ln\Gamma_k^{(i)} \right| \tag{2.73}$$

where Γ_k is the group residual activity coefficient, and $\Gamma_k^{(i)}$ is the residual activity coefficient of group k in a reference solution containing only molecules of type i. In Eq(2.73), the term $\ln\Gamma_k^{(i)}$ is necessary to attain the normalization that activity coefficient γ_i becomes unity as $X_i \rightarrow 1$. The group activity coefficient for group k in molecule i ($\Gamma_k^{(i)}$) depends on the molecule i in which k is situated. The group activity coefficient Γ_k is found from the expression :

$$\ln\Gamma_k = Q_k \left| 1 - \ln(\sum_m \Theta_m \Psi_{mk}) - \sum_m (\Theta_m \Psi_{mk} / \sum_n \Theta_n \Psi_{nm}) \right| \qquad (2.74)$$

Eq.(2.74) also holds for $\ln\Gamma_k^{(i)}$. In Eq.(2.74), Θ_m is the area fraction of group m, and the sum is over all different groups. Θ_m is calculated in a manner similar to that for θ_j :

$$\Theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n} \qquad (2.75)$$

where X_m is the mole fraction of group m in the mixture. The group interaction parameter Ψ_{mn} is given by :

$$\Psi_{mn} = \exp - \left| \frac{U_{mn} - U_{nn}}{RT} \right| = \exp - (\frac{amn}{T}) \qquad (2.76)$$

where U_{mn} is a measure of the energy of interaction between groups m and n. A sample calculation of activity coefficients with UNIFAC is given in Appendix B.

UNIFAC originally had 18 main groups and 26 subgroups (11). Later, the method was revised and its range of applicability considerably extended. (12),(13),(14).UNIFAC now encompasses 40 main groups and 76 subgroups. Although they have their own Rand Q parameters it is assumed that the subgroups within the same main group have identical group energy interaction parameters.

The limitations of UNIFAC are that it is not applied at high pressures and to systems containing noncondensable, eletrolytic and polymeric components and immiscible liquids(21).

3. COMPUTATIONAL METHODS

The thermodynamic basis for calculation of phase equilibrium conditions in PVT systems asserts that the fugacity $\hat{f}_i$ of each component i in an N-component system must be the same in all phases at equilibrium.

$$\hat{f}_i^1 = \hat{f}_i^2 = \ldots\ldots\ldots\ldots\ldots \hat{f}_i^m \qquad (3.1)$$

According to the phase rule, the number of degrees of freedom F at equilibrium is given by the difference between the number of variables and the number of equations. The variables are temperature,pressure and N mole fractions in each of the m equilibrium phases. The total number of equations are (m-1)N†m. (m-1)N of these are given by Eq.(3.1) and the rest m equation are obtained from the stoichometric relations in each phase.

$$\sum^{N} W_i = 1 \qquad (3.2)$$

where W_i is the mole fraction of component i in each phase. So, the degrees of freedom F in an N-component and inphase system at equilibrium, where total number of variables is Nm†2, can be expressed as :

$$F = 2+N-m \tag{3.3}$$

Application of Eq(3.3) to a vapor liquid equilibrium system gives $F = N$, this means that for an equilibrium state only N of the $2N+2$ variables are independent.Once,N phase rule variables are specified, remaining $N+2$ variables can be determined, in principle, by simultaneous solution of the N equilibrium relations of the form:

$$\hat{f}_i^v = \hat{f}_i^L \tag{2.2}$$

and 2 equations given by Eq.(3.2) for each phase.

Because of the engineering interest, vapor-liquid equilibrium calculations are performed by specifying either temperature or pressure, and either the liquid phase or vapor phase mole fractions. Therefore, there are four possible types of vapor-liquid equilibrium calculations as given in Table 3.1.

TABLE 3.1 The Types of VLE Calculations

Given	Find	Type
$P,X_1,X_2,..X_N$	$T,Y_1,Y_2,.Y_N$	Bubble T
$T,X_1,X_2,..X_N$	$P,Y_1,Y_2,.Y_N$	Bubble P
$P,Y_1,Y_2,..Y_N$	$T,X_1,X_2,.X_N$	Dew T
$T,Y_1,Y_2,..Y_N$	$P,X_1,X_2,.X_N$	Dew P

The equations available to perform vapor-liquid equilibrium calculations are nonlinear and to obtain a solution one must use an effective iterative procedure. For bubble and dew point calculations, two objective functions are introduced, respectively :

$$\sum_{i}^{N} k_i W_i = 1 \qquad (3.4)$$

and

$$\sum_{i}^{N} W_i / k_i = 1 \qquad (3.5)$$

with a single unknown variable either the temperature (at given pressure) or the pressure (at given temperature)(1) Here, K_i is the equilibrium ratio which is given by :

$$K_i = y_i / X_i \qquad (3.6)$$

and it can be calculated using either Eq(2.10) or Eq.(2.11)

The equations like Eq.(3.4) and (3.5) are mostly solved by an effective iteration method like Newton-Raphson method. The iteration formula of Newton-Raphson method, being essentially a point-slope method, is given by :

$$X_{new} = X_{old} - \frac{F(X_{old})}{F'(X_{old})} \qquad (3.7)$$

where X is an independent variable.

Using Raoult's law for vapor-liquid equilibrium and using Antoine equation for saturated vapor pressure, it is helpful to note that K_i tends to vary with 1/P and with exp(1/T). For bubble point temperature calculations, an objective function is redefined:

$$G(T) = \ln\left|\sum_{i=1}^{N} K_i W_i\right| = 0 \tag{3.8}$$

Similarly, for dew point temperature calculations,

$$G(1/T) = \ln\left|\sum_{i=1}^{N} W_i/K_i\right| = 0 \tag{3.9}$$

is defined. Eqs.(3.8) and (3.9) have more nearly linear behaviour than do Eqs.(3.4) and (3.5)

For bubble point and dew-point pressure calculations, the appropriate forms are, respectively :

$$G(1/P) = \sum_{i=1}^{N} K_i W_i - 1 = 0 \tag{3.10}$$

and

$$G(P) = \sum_{i=1}^{N} W_i/K_i - 1 = 0 \tag{3.11}$$

At low or moderate pressure, a Newton-Raphson iteration is not required for bubble and dew pressure calculations,and for such cases, iterations are made by using the following equations, respectively :

$$P_{new} = P_{old} \sum_{i=1} K_i W_i \tag{3.12}$$

$$P_{new} = P_{old}/(\sum_{i=1} W_i/K_i) \tag{3.13}$$

The solution of the equations in vapor-liquid equilibrium calculations, requires tedious trial and error calculations which can be effectively and easily carried out by a digital computer. The interactive computer program VLENC written in Fortran V, in this study, has mainly four options for vapor-liquid equilibrium calculations: DewT,Bubble T, Dew P and Bubble P as given in Table 3.1, for the multicomponent systems containing condensable and noncondensable components. VLENC calculates vapor-phase nonidealities using Peng-Robinson equation, but it has two options for liquid phase nonideality, namely UNIQUAC and UNIFAC. VLENC consists of a main program and 17 subroutines. The relations between main program and its subroutines are given in Figure 1. VLENC also contains 4 data files : YLIST is used for the names of the components for which thermophysical properties exists, YDATAPP is used for the physical properties of those components, YDATAUQ and YDATUM are used, respectively for the parameters of UNIQUAC and the functional group parameters of UNIFAC equations. The list of the UNIFAC and UNIQUAC parameters are given in Appendix C.

The flow diagrams of the subroutines DEW T, DEW P, BUB. T, BUB. P are given in figures (3.2),(3.3),(3.4). The flow diagrams for the Dew T and Bubble T calculations are given on the same figure, because the same procedure is used for both calculations. DEWT is one of the main subroutines of VLENC for the calculation of dew-point temperature of a multicomponent mixture. In the prediction of dew point temperature, the program tries to equate the objective function, G given by Eq(3.9), to zero.

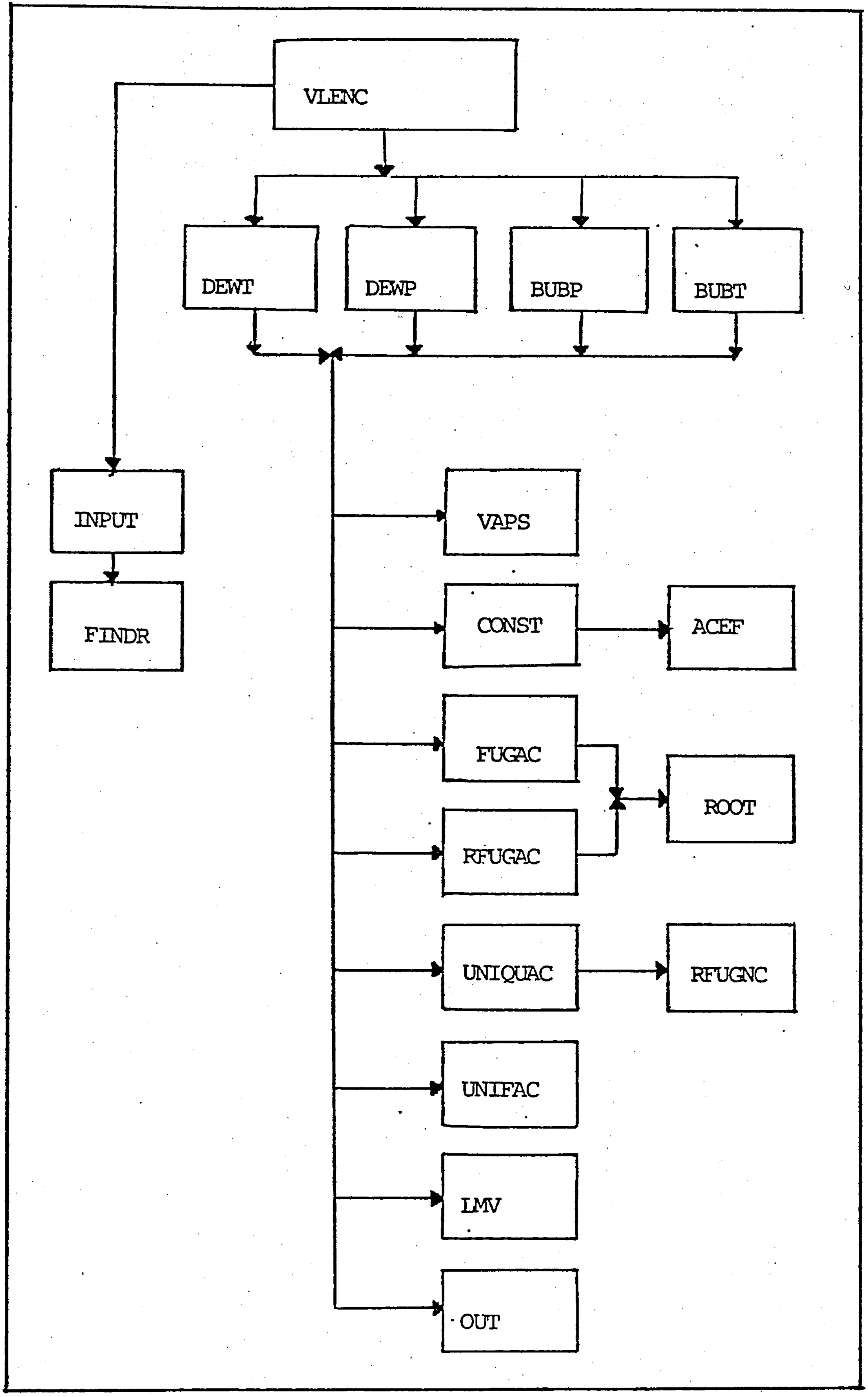

FIGURE 3.1 Program VLENC and its Subroutines

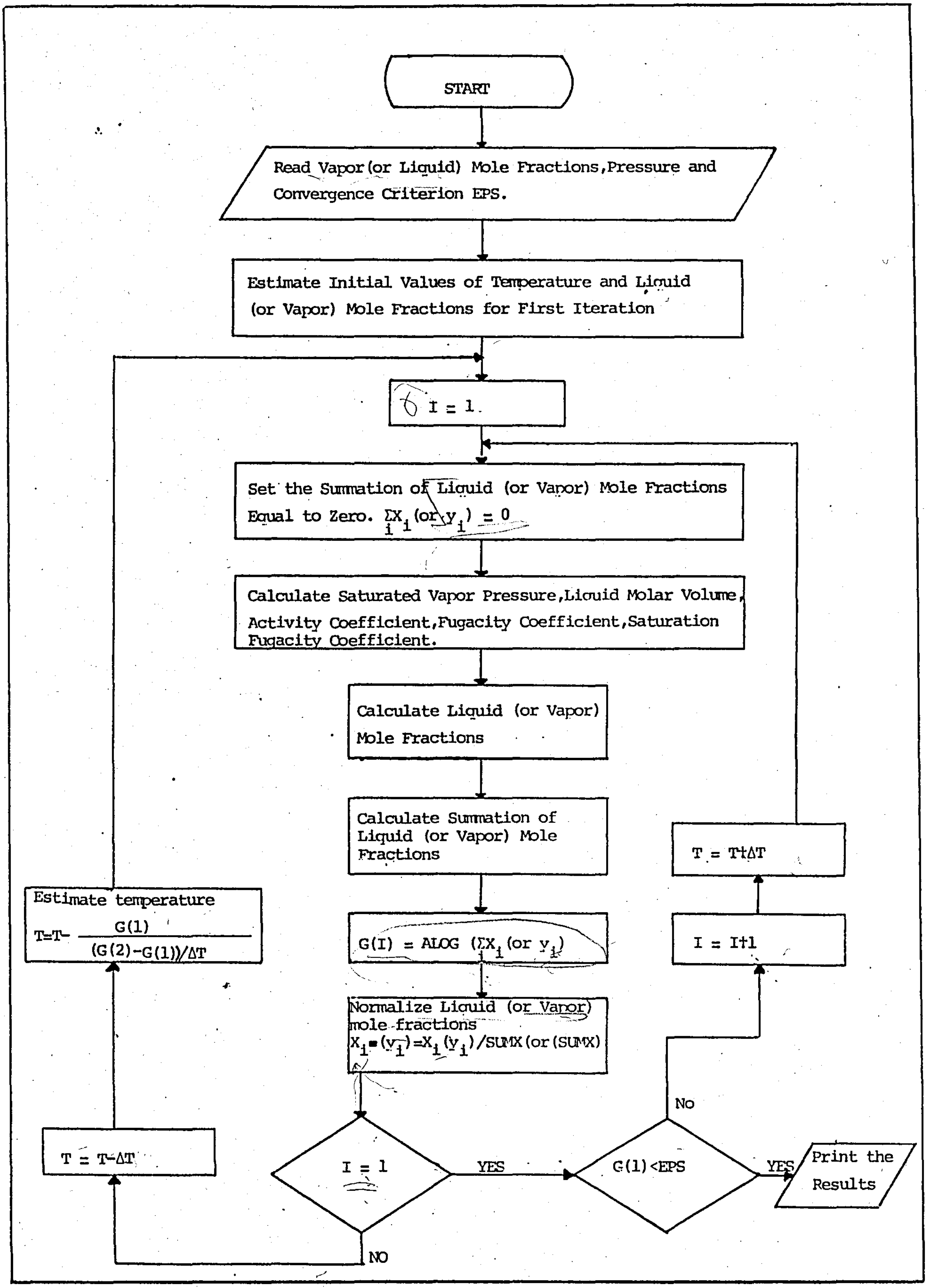

FIGURE 3.2. Flow Diagram for DewT (program DEWT) and BubbleT (Program BUBT) Calculations

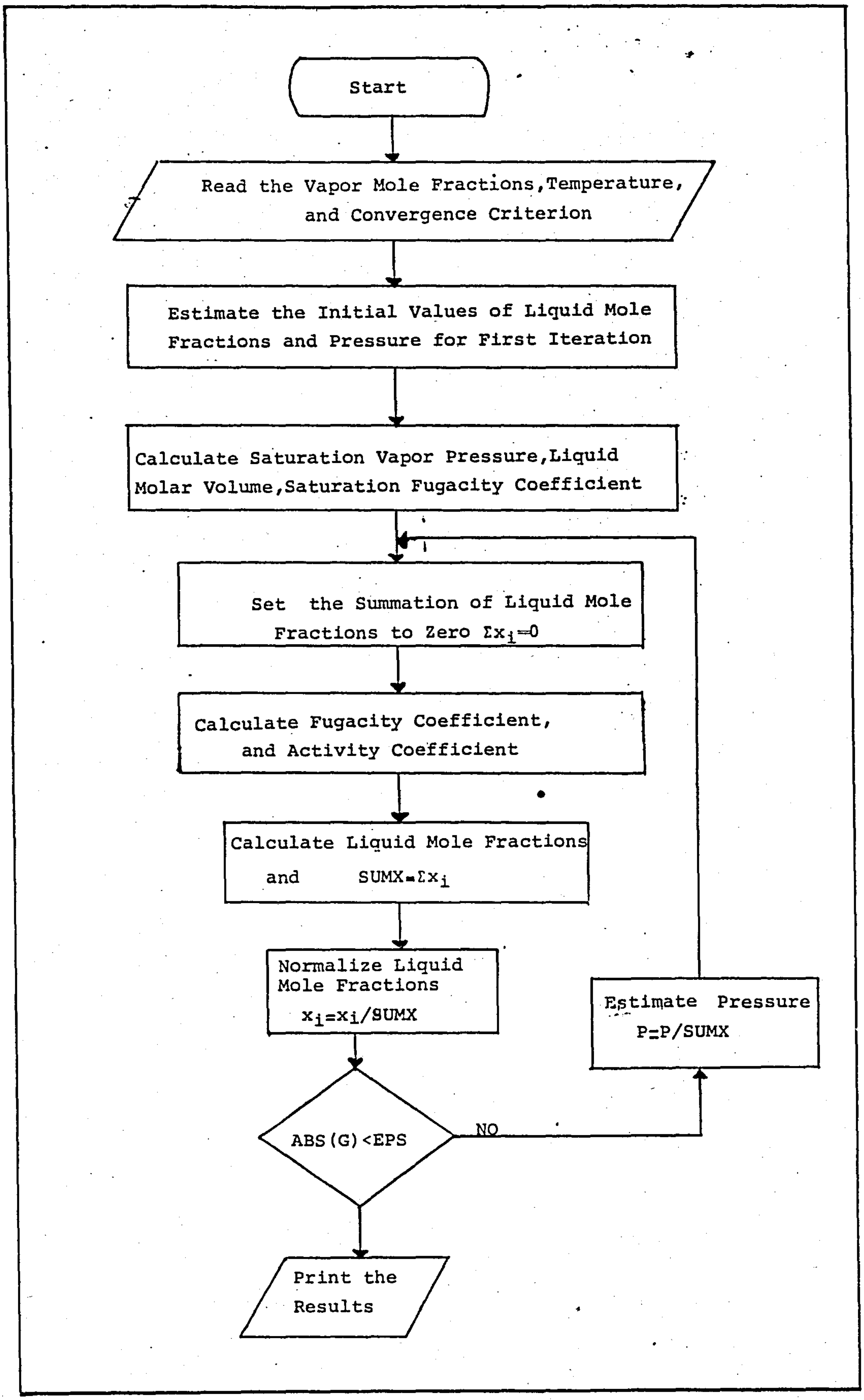

FIGURE 3.3. Flow Diagram for Dew P Calculations(Program DEWP)

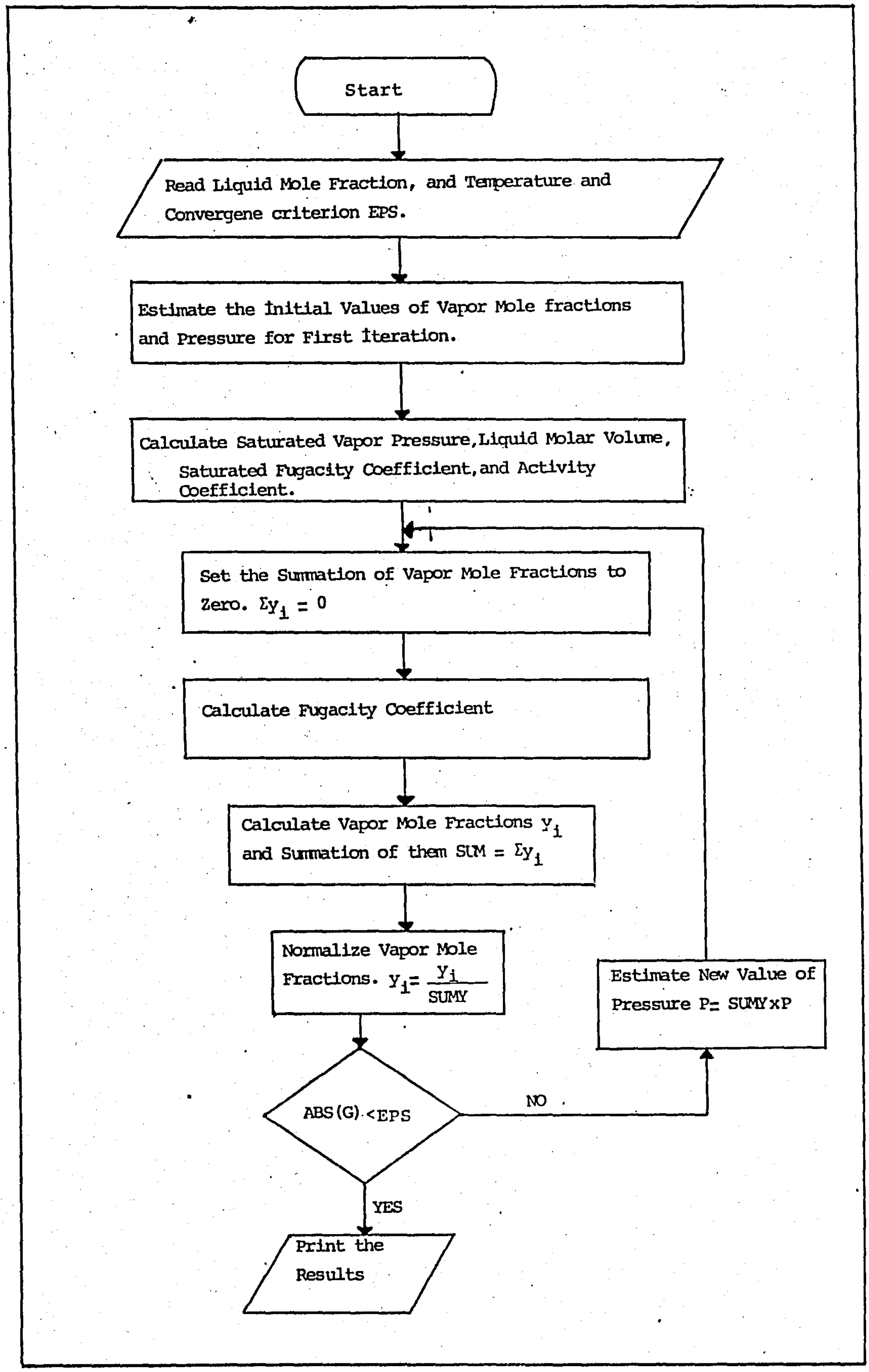

FIGURE 3.4. Flow Diagram for Bubble P Calculations (Program BUBP)

After reading vapor-mole fractions and pressure, the program estimates the temperature and liquid mole fractions for first iteration (Fig.(3.2)). Next, the program enters an iterative loop and following the calculations of the thermodynamic functions required in vapor-liquid equilibria, it estimates liquid mole fractions by applying Eq.(2.11) for the condensable components or Eq.(2.10) for noncondensable components. Then, the program calculates the objective function G, and normalizes predicted liquid mole fractions. Before repeating calculations for G at $T+\Delta T$ in Newton-Raphson formulation, it compares the function G at T with convergence criterion EPS. Next, it finds a new valu of temperature for other iterations in Newton-Raphson formulation. All thermodynamic functions have to be recalculated for each temperature because of their temperature dependence. This iterative calculational procedure continues until the value of the objective function G becomes less than EPS. In this case, the program prints the results and stops.

The subroutine BUBT calculates bubble point temperature conditions. Calculational procedure of BUBT is the same as the procedure of DEWT and flow diagram can also be represented as given in Fig(3.2). In this case only, the notation of the mole fractions are different as given in parenthesis.

The subroutine DEWP, is the third main subroutine of the main program VLENC and is able to perform dew point pressure calculations (Fig.(3.3)). Program reads vapor compositions and temperature, and estimates the initial values of pressure and liquid mole fractions. Then, it calculates saturated vapor pressure P_i^S, liquid molar volume V_i^L , and saturated fugacity coefficient ϕ_i^S , required in the prediction of liquid compositions. Since these functions are independent of pressure, they are not calculated for each additional pressure estimation. Next, the program enters into iterative scheme. After calculating fugacity coefficient $\hat{\phi}_i$, which is a function of P, and activity coefficient γ_i, which is a function of liquid mole fraction, the liquid mole fractions are predicted. Program normalizes the liquid mole fractions and compares the objective function for dew pressure (Eq.3.11) with the convergence criterion EPS. If the value of the difference is greater than EPS, it estimates the new value of pressure for next iteration using Eq. (3.13). Because of the linear behaviour of dew pressure or bubble pressure objective functions, Newton-Raphson iterative technique is not required to avoid unnecessary calculations. Iteration continues until objective function becomes less than EPS.

Last option of vapor-liquid calculations,bubble point pressure, is performed by the subroutine BUBP.The program reads temperature and liquid mole fractions (Fig 3.4). Next, it calculates all thermodynamic functions which are not functions of pressure and vapor mole fractions, except fugacity coefficient, which depends on pressure and vapor mole fractions. Then iterative scheme comes and only fugacity coefficient calculation takes place in this loop. After calculating vapor mole fractions, it compares the objective function for bubble point pressure with the convergence criterion, EPS (Eq.3.10) Unless the objective function G, reaches a value less than EPS, it continues iterations by estimating a new value of pressure by Eq.(3.12).

The detalied description and listing of the programs are given in Appendix C.

4. RESULTS AND DISCUSSION

In this work, thirty three binary and four ternary systems were studied. Besides comparing the experimental and calculated results, UNIQUAC and UNIFAC results were compared with each other. For this purpose systems were selected such that the required parameters for the calculation of vapor-liquid equilibria are available in both UNIQUAC and UNIFAC parameter tables.

The program VLENC have been run for about 1500 data points. Because of the large number of calculations, some of the results are given as average absolute mean deviations from experimental data for the whole data set. Average absolute mean deviation (AMD) is calculated by :

$$\text{AMD} = \frac{\sum_{1}^{N} \text{ABS}\ (G_{\text{calculated}} - G_{\text{experimental}})}{N}$$

where G is any variable such as X,y,T or P, and N is the number of data points. Most of the calculations performed were bubble T and dew T type because, in literature, most experimental data are available at isobaric conditions. First thirty tables give the computational results for binary and ternary systems for each experimental point. In Tables 4.1-4.30, for each system equilibrium results are given for both UNIQUAC and UNIFAC equations.

UNIQUAC and UNIFAC pure component and interaction parameters are presented in Appendix C. Even though for UNIQUAC, sometimes more than one interaction parameter is encountered in literature for a binary pair, in this work only one which gives best results for the system studied, is presented in the tables and in the data file.

Tables 4.1-4.4 presents dewT and bubbleT predictions of i-Propanol-2,2,4-Trimethyl pentane binary system. As it is seen in Tables 4.1 and 4.2, bubbleT predictions for that system performed by UNIQUAC are much better than by UNIFAC. Tables 4.3,4.4 give us the DewT results of the same system using UNIQUAC and UNIFAC, respectively. Here, also, the results obtained by UNIQUAC, although not as good as in the case of bubbleT predictions, are in better agreement with experimental results than those predicted by UNIFAC.

Tables 4.5-4.8 present the bubbleP and dewP predictions for the 2,2,4-trimethyl pentane and toluene binary system. In this case, the predictions by UNIFAC are slightly better than those of UNIQUAC. Also, for this system, dew point predictions are worser than bubble point predictions.

Tables 4.9-4.14 show that the phase equilibrium predictions for n-hexane-ethanol, n-hexane-benzene and n-hexane-toluene binary systems by either UNIQUAC or UNIFAC equations are quite good.

Bubble point predictions for benzene i-propanol system by either UNIQUAC or UNIFAC, as it is seen in Tables 4.15 and 4.16, are in very good agreement with the experimental data.

By comparing Tables 4.17 and 4.18, it is observed that the predicted bubbleT results by UNIFAC for methanol-2-butanone system is very good and better than the results predicted by UNIQUAC. For this system, UNIQUAC interaction parameters obtained from experimental data in literature, should be rechecked.

In Tables 4.19-4.22, dewT and bubbleT results, respectively, for the binary systems of water-ethanol and water-methanol are given. Average mean deviations of liquid mole fractions, vapor mole fractions and temperature show that the results predicted either by UNIQUAC or UNIFAC, are in good agreement with the experimental VLE data.

In Tables 4.23-4.30, results of three different ternary systems are presented. The ternary systems contain components which are considered in the preceeding tables. In Tables 4.23 and 4.24 bubbleT predictions for acetone-methanol-water ternary system are given. The absolute mean deviations in $y_i^{'}$ s of the components are 0.0121,0.0066,0.0068 for acetone, methanol,water,respectively, and absolute mean deviation in temperature is 0.8002 by using UNIQUAC. Although the predictions by UNIFAC are not as good as those obtained by UNIQUAC they are still in good agreement with experimental data.

Comparison of Tables 4.25 and4.26 shows that for 2-butanone-n-heptane-toluene ternary system, also UNIQUAC predictions are better than those obtained UNIFAC.

The last ternary system whose results are tabulated point by point, is the methanol-carbon tetrachloride-benzene system. As it is seen from Tables 4.27 and 4.28 bubbleP calculation by UNIQUAC gives excellent results. The mean deviation in pressure is 0.014 atm, which is quite acceptable for a system pressure of about 0.9 atm. The results obtained at the same conditions by UNIFAC, are worser than those obtained by UNIQUAC. The absolute mean deviations in y_i' and in pressure are about 10 times of those obtained with UNIQUAC.

Tables 4.29 and 4.30 give the results of dewT calculations for the previous system. As observed in previous cases, dew point predictions by UNIQUAC are not as good as bubble point predictions. However, in this case, UNIFAC dew point predictions are slightly better than UNIFAC bubble point predictions.

In the next six tables, Tables 4.31-4.36, the predictions are given on the basis of whole data set for each system. In these tables, experimental data are compared with the calculated results using UNIQUAC, UNIFAC and Raoult's law.

The computational results are given as absolute mean deviations both in compositions and in temperature or in pressure, for the whole data set of each system. It is seen that the results obtained by either of UNIQUAC and UNIFAC are in much better agreement with experimental data than obtained by Raoult's law.

Table 4.31 presents VLE calculation results for the binary systems containing various alcohols and aromatics. It is seen that VLE calculations by UNIQUAC give an average absolute mean deviation of 0.0309 in y_i's. This is an acceptable error. In the case of calculations by UNIFAC, average absolute mean of 0.0205 in y_i's is obtained. This is slightly better than that obtained by UNIQUAC. Largest errors are encountered in dew pressure calculations. The temperatures and pressures predicted both by UNIFAC and UNIQUAC are quite acceptable.

In Table 4.33, one observes that the VLE predictions for alkane-alcohol systems by UNIQUAC and UNIFAC, range from good to moderate.

Table 4.32 shows that the VLE predictions for the binary systems containing alkanes and aromatics yield quite low absolute mean deviations. These are the smallest absolute mean deviations obtained among all systems studied in this work.

In Tables, 4.34 and 4.35, VLE predictions are given for alcohol-water and ketone-alcohol binary systems, respectively. The absolute mean deviations in compositions and in temperature exhibit moderate errors for both of UNIQUAC and UNIFAC. Only for methanol-2-butanone system, large deviations are observed when UNIQUAC is used.

The VLE predictions for ternary systems run in this work, are tabulated in Table 4.36. The results of some of these systems are given in previous tables point by point. As it is seen, the VLE predictions for ternary systems give acceptable errors, although not as good as binary systems. But,for water-formic acid-acetic acid system the predictions are not too good, especially when UNIFAC is used. In this case, results obtained by UNIFAC are comparable to those obtained by Raoult's law.

Tables 4.37-4.39 give VLE predictions for ethanol-water, acetone-water, and methanol-water systems at various pressures. It can be seen that although the errors slightly increase with increase in pressure, they are in the acceptable limits. At low pressures, the fugacity coefficient does not go below 0.95. It is mostly around 0.98 or very close to unity. So, at low pressures, vapor phase can be assumed to be ideal. But at higher pressures, higher vapor phase nonidealities are obtained and thus, use of Peng-Robinson equation in VLE calculations, is justified.

In Tables 4.40 and 4.43, bubbleT results for acetone-water and ethanol-water binaries are given for quite high pressures.Since the pressures are high, fugacity coefficients take on values of 0.81 or above. In order to show the influence of pressure and thus of fugacity coefficients, in Tables 4.44 and 4.45, the absolute mean deviations for methanol-water and acetone-water binary systems at various pressures, are compared with those values obtained by using ideal gas assumption. The last column presents the difference in absolute mean deviations obtained by Peng-Robinson equation and ideal gas equation.

In this study, the aim was to develop a computer program to do VLE calculations for multicomponent systems and then to search for the applicability of UNIFAC and UNIQUAC equations for various systems with available experimental data.Comparision of all results show that bubble point predictions are better than dew point predictions. Dew P predictions are not as good as the others.

Finally, it can be said that the VLE predictions for the systems studied in this work containing condensable components, generally show good agreement with experimental data except for a few systems. Although agreement between the results predicted by UNIFAC and UNIQUAC are observed in general UNIQUAC gives better results for ternary systems studied.

Even though the influence of vapor phase nonideality is not much at low pressure, it must be considered for accurate design calculations in the case of pressures above a few atmospheres.

Unfortunately, the results for the systems containing noncondensable components are not encouraging. In Tables 4.46 and 4.47, the predictions are presented for two binary systems, where one of the components is noncondensable. The predictions nitrogen-n-butane system shows that as the composition of noncondensable component in liquid phase goes to zero, the deviations in composition and in pressure becomes very small. This is expected because the equations used here are for noncondensable components at infinite dilution. Predictions of hydrogen-n-hexane system are quite good for vapor-phase composition but not for pressures. Thus, for systems containing noncondensables, the results are not as good as those obtained for systems containing only condensables.

TABLE 4.1. Bubble T Results for i-Propanol(1)-2,2,4 Trimethyl Pentane(2) System Using UNIQUAC(15).

```
 PRESSURE=   1.000  ATM

                 GIVEN                                   CALCULATED
          --------------------    ---------------------------------------------
DATA COMP    X      YE       TE        T         GAMA       FHI        Y
*****************************************************************************
  1   1   .0290  .1770   366.65   365.87     4.3765     .9670     .1864
      2   .9710  .8230                       1.0016     .9522     .8136
  2   1   .0580  .2930   362.55   361.79     3.9934     .9652     .2939
      2   .9420  .7070                       1.0065     .9508     .7061
  3   1   .1210  .4350   356.75   356.83     3.2779     .9631     .4187
      2   .8790  .5650                       1.0277     .9491     .5813
  4   1   .2300  .5260   353.35   353.17     2.4361     .9616     .5141
      2   .7700  .4740                       1.0960     .9478     .4859
  5   1   .3310  .5550   352.25   351.72     1.9495     .9609     .5595
      2   .6690  .4450                       1.1959     .9473     .4405
  6   1   .3905  .5730   351.75   351.23     1.7430     .9607     .5789
      2   .6095  .4270                       1.2740     .9471     .4211
  7   1   .5170  .6020   350.95   350.65     1.4278     .9604     .6134
      2   .4830  .3980                       1.5036     .9470     .3866
  8   1   .6130  .6300   350.75   350.46     1.2644     .9603     .6394
      2   .3870  .3700                       1.7608     .9469     .3606
  9   1   .6765  .6545   350.45   350.45     1.1820     .9603     .6594
      2   .3235  .3455                       1.9900     .9470     .3406
 10   1   .8000  .7200   351.25   350.85     1.0684     .9605     .7160
      2   .2000  .2800                       2.6513     .9473     .2840
 11   1   .8780  .7800   351.55   351.67     1.0250     .9608     .7789
      2   .1220  .2200                       3.2993     .9479     .2211
 12   1   .9575  .8950   353.35   353.58     1.0029     .9618     .8951
      2   .0425  .1050                       4.2377     .9495     .1049

          ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=    .0067

          ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=    .35
------------------------------------------------------------------------------
```

TABLE 4.2. Bubble T Results for i-Propanol(1)-2,2,4 Trimethyl Pentane(2) System Using UNIFAC(15).

```
 PRESSURE=   1.000  ATM

                 GIVEN                                   CALCULATED
          --------------------    ---------------------------------------------
DATA COMP    X      YE       TE        T         GAMA       FHI        Y
*****************************************************************************
  1   1   .0290  .1770   366.65   360.72     8.3801     .9648     .2966
      2   .9710  .8230                       1.0033     .9504     .7034
  2   1   .0580  .2930   362.55   355.44     7.0768     .9626     .4111
      2   .9420  .7070                       1.0128     .9485     .5889
  3   1   .1210  .4350   356.75   350.86     4.9791     .9606     .5048
      2   .8790  .5650                       1.0510     .9468     .4952
  4   1   .2300  .5260   353.35   348.79     3.1005     .9597     .5502
      2   .7700  .4740                       1.1633     .9460     .4498
  5   1   .3310  .5550   352.25   348.32     2.2500     .9595     .5638
      2   .6690  .4450                       1.3180     .9459     .4362
  6   1   .3905  .5730   351.75   348.19     1.9336     .9594     .5688
      2   .6095  .4270                       1.4358     .9458     .4312
  7   1   .5170  .6020   350.95   348.04     1.4934     .9594     .5800
      2   .4830  .3980                       1.7736     .9458     .4200
  8   1   .6130  .6300   350.75   348.01     1.2957     .9593     .5940
      2   .3870  .3700                       2.1419     .9458     .4060
  9   1   .6765  .6545   350.45   348.09     1.1995     .9594     .6087
      2   .3235  .3455                       2.4632     .9459     .3913
 10   1   .8000  .7200   351.25   348.78     1.0738     .9596     .6626
      2   .2000  .2800                       3.3619     .9463     .3374
 11   1   .8780  .7800   351.55   350.02     1.0275     .9601     .7314
      2   .1220  .2200                       4.2192     .9470     .2686
 12   1   .9575  .8950   353.35   352.77     1.0034     .9614     .8680
      2   .0425  .1050                       5.4682     .9489     .1320

          ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=    .0485

          ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=   3.63
------------------------------------------------------------------------------
```

TABLE 4.3. Dew T Results for i-Propanol(1)-2,2,4 Trimethyl Pentane(2) System Using UNIQUAC(15).

```
     PRESSURE=   1.000 ATM

                     GIVEN                                   CALCULATED
             -------------------     ------------------------------------------
DATA COMP    Y       XE       TE        T          GAMA       FHI          X
*******************************************************************************
  1   1    .1770   .0290    366.65    366.22      4.4026     .9671      .0270
      2    .8230   .9710                          1.0014     .9523      .9730
  2   1    .2930   .0580    362.55    361.83      3.9911     .9653      .0578
      2    .7070   .9420                          1.0065     .9508      .9422
  3   1    .4350   .1210    356.75    356.18      3.1490     .9629      .1341
      2    .5650   .8790                          1.0340     .9488      .8659
  4   1    .5260   .2300    353.35    352.76      2.3000     .9614      .2533
      2    .4740   .7700                          1.1165     .9476      .7467
  5   1    .5550   .3310    352.25    351.85      1.9882     .9610      .3204
      2    .4450   .6690                          1.1845     .9473      .6796
  6   1    .5730   .3905    351.75    351.37      1.7948     .9608      .3733
      2    .4270   .6095                          1.2511     .9472      .6267
  7   1    .6020   .5170    350.95    350.80      1.5128     .9605      .4760
      2    .3980   .4830                          1.4201     .9470      .5240
  8   1    .6300   .6130    350.75    350.50      1.3227     .9604      .5764
      2    .3700   .3870                          1.6484     .9469      .4236
  9   1    .6545   .6765    350.45    350.44      1.2036     .9603      .6596
      2    .3455   .3235                          1.9138     .9470      .3404
 10   1    .7200   .8000    351.25    350.39      1.0651     .9605      .8055
      2    .2800   .2000                          2.6842     .9474      .1945
 11   1    .7800   .8780    351.55    351.69      1.0250     .9608      .8787
      2    .2200   .1220                          3.2995     .9479      .1213
 12   1    .8950   .9575    353.35    353.58      1.0029     .9618      .9574
      2    .1050   .0425                          4.2366     .9495      .0426

                  ERROR ON X(1)= ABS(X(1)-XE(1))/DATA POINTS=    .01391

                  ERROR ON T= ABS(TE-T)/DATA POINTS=   .35
-------------------------------------------------------------------------------
```

TABLE 4.4. Dew T results for i-Propanol(1)-2,2,4 Trimethyl Pentane(2) System Using UNIFAC(15).

```
     PRESSURE=   1.000 ATM

                     GIVEN                                   CALCULATED
             -------------------     ------------------------------------------
DATA COMP    Y       XE       TE        T          GAMA       FHI          X
*******************************************************************************
  1   1    .1770   .0290    366.65    365.74      9.0816     .9669      .0133
      2    .8230   .9710                          1.0007     .9521      .9867
  2   1    .2930   .0580    362.55    360.88      8.3996     .9649      .0284
      2    .7070   .9420                          1.0032     .9505      .9716
  3   1    .4350   .1210    356.75    354.29      6.6286     .9621      .0685
      2    .5650   .8790                          1.0178     .9481      .9315
  4   1    .5260   .2300    353.35    349.85      4.1710     .9602      .1567
      2    .4740   .7700                          1.0825     .9464      .8433
  5   1    .5550   .3310    352.25    348.60      2.7317     .9596      .2653
      2    .4450   .6690                          1.2132     .9460      .7347
  6   1    .5730   .3905    351.75    348.12      1.6629     .9594      .4589
      2    .4270   .6095                          1.6054     .9458      .5411
  7   1    .6020   .5170    350.95    348.04      1.2450     .9594      .6458
      2    .3980   .4830                          2.2914     .9458      .3542
  8   1    .6300   .6130    350.75    348.31      1.1311     .9594      .7360
      2    .3700   .3870                          2.8348     .9460      .2640
  9   1    .6545   .6765    350.45    348.65      1.0857     .9596      .7856
      2    .3455   .3235                          3.2246     .9462      .2144
 10   1    .7200   .8000    351.25    349.80      1.0328     .9601      .8674
      2    .2800   .2000                          4.0750     .9469      .1326
 11   1    .7800   .8780    351.55    350.99      1.0141     .9606      .9131
      2    .2200   .1220                          4.7099     .9476      .0869
 12   1    .8950   .9575    353.35    353.32      1.0019     .9617      .9679
      2    .1050   .0425                          5.6702     .9494      .0321

                  ERROR ON X(1)= ABS(X(1)-XE(1))/DATA POINTS=    .06491

                  ERROR ON T= ABS(TE-T)/DATA POINTS=  2.08
-------------------------------------------------------------------------------
```

TABLE 4.5. Bubble P Results for 2,2,4 Trimethyl Pentane(1) - Toluene (2) System Using UNIQUAC(15).

```
     TEMPERATURE=  373.15  K

                      GIVEN                                    CALCULATED
               --------------------    ----------------------------------------
DATA  COMP     X       YE       PE        P           GAMA      FHI       Y
*******************************************************************************
  1    1     .1000   .1700     .795      .785       1.2035    .9649     .1548
       2     .9000   .8300                          1.0041    .9728     .8452
  2    1     .2000   .2999     .847      .826       1.1356    .9629     .2781
       2     .8000   .7001                          1.0143    .9714     .7219
  3    1     .3000   .4049     .889      .861       1.0889    .9613     .3846
       2     .7000   .5951                          1.0284    .9703     .6154
  4    1     .4000   .4945     .922      .891       1.0566    .9599     .4815
       2     .6000   .5055                          1.0451    .9693     .5185
  5    1     .5000   .5754     .949      .918       1.0344    .9588     .5728
       2     .5000   .4246                          1.0633    .9686     .4272
  6    1     .6000   .6437     .969      .942       1.0194    .9577     .6608
       2     .4000   .3563                          1.0823    .9679     .3392
  7    1     .7000   .7319     .985      .964       1.0097    .9569     .7469
       2     .3000   .2681                          1.1016    .9674     .2531
  8    1     .8000   .8201     .998      .984       1.0039    .9564     .8318
       2     .2000   .1799                          1.1209    .9672     .1682
  9    1     .9000   .9102    1.010     1.001       1.0009    .9569     .9160
       2     .1000   .0898                          1.1398    .9676     .0840

            ERROR ON Y(1)= ABS(YE(1)-Y(1)/DATA POINTS=    .0136

            ERROR ON P= ABS(PE-P)/DATA POINTS=     .022
-------------------------------------------------------------------------------
```

TABLE 4.6. Bubble P Results for 2,2,4 Trimethyl Pentane(1) - Toluene (2) System Using UNIFAC(15).

```
     TEMPERATURE=  373.15  K

                      GIVEN                                    CALCULATED
               --------------------    ----------------------------------------
DATA  COMP     X       YE       PE        P           GAMA      FHI       Y
*******************************************************************************
  1    1     .1000   .1700     .795      .807       1.4078    .9639     .1763
       2     .9000   .8300                          1.0056    .9720     .8237
  2    1     .2000   .2999     .847      .863       1.2895    .9613     .3030
       2     .8000   .7001                          1.0212    .9701     .6970
  3    1     .3000   .4049     .889      .905       1.2011    .9593     .4042
       2     .7000   .5951                          1.0455    .9688     .5958
  4    1     .4000   .4945     .922      .939       1.1352    .9578     .4919
       2     .6000   .5055                          1.0777    .9677     .5081
  5    1     .5000   .5754     .949      .966       1.0866    .9566     .5730
       2     .5000   .4246                          1.1169    .9669     .4270
  6    1     .6000   .6437     .969      .987       1.0515    .9557     .6518
       2     .4000   .3563                          1.1625    .9664     .3482
  7    1     .7000   .7319     .985     1.003       1.0270    .9551     .7315
       2     .3000   .2681                          1.2142    .9661     .2685
  8    1     .8000   .8201     .998     1.013       1.0113    .9550     .8145
       2     .2000   .1799                          1.2717    .9661     .1855
  9    1     .9000   .9102    1.010     1.019       1.0027    .9558     .9032
       2     .1000   .0898                          1.3346    .9668     .0968

            ERROR ON Y(1)= ABS(YE(1)-Y(1)/DATA POINTS=    .0040

            ERROR ON P= ABS(PE-P)/DATA POINTS=     .015
-------------------------------------------------------------------------------
```

TABLE 4.7. Dew P Results for 2,2,4 Trimethyl Pentane(1)-Toluene(2) System Using UNIQUAC(15).

```
        TEMPERATURE= 373.15 K

                         GIVEN                                              CALCULATED
                  --------------------     --------------------------------------------
DATA  COMP      Y       XE         PE           P             GAMA        FHI          X
***************************************************************************************
   1    1     .1700   .1000       .795         .789          1.1944      .9647       .1114
        2     .8300   .9000                                  1.0050      .9726       .8886
   2    1     .2999   .2000       .847         .833          1.1250      .9626       .2196
        2     .7001   .8000                                  1.0168      .9712       .7804
   3    1     .4049   .3000       .889         .867          1.0813      .9610       .3204
        2     .5951   .7000                                  1.0317      .9701       .6796
   4    1     .4945   .4000       .922         .894          1.0529      .9598       .4140
        2     .5055   .6000                                  1.0476      .9692       .5860
   5    1     .5754   .5000       .949         .918          1.0339      .9587       .5029
        2     .4246   .5000                                  1.0639      .9686       .4971
   6    1     .6437   .6000       .969         .937          1.0219      .9579       .5804
        2     .3563   .4000                                  1.0786      .9681       .4196
   7    1     .7319   .7000       .985         .960          1.0111      .9571       .6825
        2     .2681   .3000                                  1.0932      .9675       .3175
   8    1     .8201   .8000       .998         .981          1.0045      .9565       .7862
        2     .1799   .2000                                  1.1182      .9672       .2138
   9    1     .9102   .9000      1.010        1.000          1.0010      .9568       .8931
        2     .0898   .1000                                  1.1385      .9675       .1069

              ERROR ON X(1)= ABS(XE(1)-X(1))/DATA POINTS=    .0140

              ERROR ON PRESSURE= ABS(PE-P)/DATA POINTS=    .021
---------------------------------------------------------------------------------------
```

TABLE 4.8. Dew P Results for 2,2,4 Trimethyl Pentane(1)-Toluene(2) System Using UNIFAC(15).

```
        TEMPERATURE= 373.15 K

                         GIVEN                                              CALCULATED
                  --------------------     --------------------------------------------
DATA  COMP      Y       XE         PE           P             GAMA        FHI          X
***************************************************************************************
   1    1     .1700   .1000       .795         .789          1.2213      .9647       .1088
        2     .8300   .9000                                  1.0014      .9726       .8912
   2    1     .2999   .2000       .847         .836          1.1932      .9625       .2078
        2     .7001   .8000                                  1.0059      .9710       .7922
   3    1     .4049   .3000       .889         .877          1.1662      .9606       .3004
        2     .5951   .7000                                  1.0138      .9697       .6996
   4    1     .4945   .4000       .922         .913          1.1395      .9590       .3900
        2     .5055   .6000                                  1.0263      .9686       .6100
   5    1     .5754   .5000       .949         .944          1.1126      .9576       .4801
        2     .4246   .5000                                  1.0455      .9677       .5199
   6    1     .6437   .6000       .969         .970          1.0880      .9565       .5633
        2     .3563   .4000                                  1.0714      .9669       .4367
   7    1     .7319   .7000       .985         .998          1.0555      .9553       .6786
        2     .2681   .3000                                  1.1266      .9662       .3214
   8    1     .8201   .8000       .998        1.018          1.0263      .9548       .7970
        2     .1799   .2000                                  1.2206      .9660       .2030
   9    1     .9102   .9000      1.010        1.025          1.0063      .9557       .9092
        2     .0898   .1000                                  1.3716      .9667       .0908

              ERROR ON X(1)= ABS(XE(1)-X(1))/DATA POINTS=    .0130

              ERROR ON PRESSURE= ABS(PE-P)/DATA POINTS=    .010
---------------------------------------------------------------------------------------
```

TABLE 4.9. Bubble T Results for n-Hexane(1)-Ethanol(2) System Using UNIQUAC(15)

```
 PRESSURE=    1.000  ATM

                   GIVEN                                       CALCULATED
           --------------------   -----------------------------------------
DATA COMP    X      YE       TE        T           GAMA      FHI       Y
***************************************************************************
  1   1    .0930  .4740   338.21    337.63       5.7808    .9586    .4717
      2    .9070  .5260                          1.0239    .9767    .5283
  2   1    .1898  .5900   334.16    333.75       3.8995    .9571    .5752
      2    .8102  .4100                          1.0904    .9763    .4248
  3   1    .2965  .6140   332.89    332.24       2.8110    .9566    .6172
      2    .7035  .3860                          1.2098    .9762    .3828
  4   1    .3885  .6350   332.17    331.70       2.2474    .9564    .6353
      2    .6115  .3650                          1.3587    .9761    .3647
  5   1    .4999  .6460   331.83    331.39       1.8019    .9562    .6490
      2    .5001  .3540                          1.6208    .9762    .3510
  6   1    .5988  .6570   331.67    331.28       1.5317    .9562    .6584
      2    .4012  .3430                          1.9764    .9762    .3416
  7   1    .6930  .6710   331.54    331.26       1.3417    .9562    .6671
      2    .3070  .3290                          2.5191    .9762    .3329
  8   1    .8021  .6760   331.68    331.39       1.1765    .9563    .6799
      2    .1979  .3240                          3.7363    .9763    .3201
  9   1    .9084  .7150   332.56    332.04       1.0575    .9565    .7068
      2    .0916  .2850                          7.1838    .9766    .2932

           ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=    .0046

           ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=    .45
---------------------------------------------------------------------------
```

TABLE 4.10. Bubble T Results for n-Hexane(1)-Ethanol(2) System Using UNIFAC(15)

```
 PRESSURE=    1.000  ATM

                   GIVEN                                       CALCULATED
           --------------------   -----------------------------------------
DATA COMP    X      YE       TE        T           GAMA      FHI       Y
***************************************************************************
  1   1    .0930  .4740   338.21    339.38       5.0510    .9593    .4350
      2    .9070  .5260                          1.0164    .9769    .5650
  2   1    .1898  .5900   334.16    334.50       3.7728    .9574    .5700
      2    .8102  .4100                          1.0680    .9764    .4300
  3   1    .2965  .6140   332.89    332.38       2.8450    .9566    .6274
      2    .7035  .3860                          1.1709    .9763    .3726
  4   1    .3885  .6350   332.17    331.67       2.2935    .9563    .6491
      2    .6115  .3650                          1.3094    .9762    .3509
  5   1    .4999  .6460   331.83    331.38       1.8338    .9562    .6603
      2    .5001  .3540                          1.5697    .9762    .3397
  6   1    .5988  .6570   331.67    331.34       1.5405    .9562    .6634
      2    .4012  .3430                          1.9426    .9762    .3366
  7   1    .6930  .6710   331.54    331.34       1.3327    .9562    .6642
      2    .3070  .3290                          2.5332    .9762    .3358
  8   1    .8021  .6760   331.68    331.39       1.1566    .9563    .6684
      2    .1979  .3240                          3.8710    .9763    .3316
  9   1    .9084  .7150   332.56    332.25       1.0418    .9566    .7009
      2    .0916  .2850                          7.2616    .9767    .2991

           ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=    .0151

           ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=    .46
---------------------------------------------------------------------------
```

TABLE 4.11. Dew T Results for n-Hexane(1)-Benzene(2) System Using UNIQUAC(15)

```
PRESSURE=    1.000 ATM

                   GIVEN                                     CALCULATED
             -------------------    --------------------------------------------
DATA COMP    Y      XE       TE        T           GAMA       FHI         X
*******************************************************************************
  1   1    .1400  .0730    350.75   350.71       1.4594     .9623      .0744
      2    .8600  .9270                          1.0030     .9707      .9256
  2   1    .2680  .1720    348.25   348.43       1.3444     .9615      .1648
      2    .7320  .8280                          1.0144     .9703      .8352
  3   1    .3760  .2680    346.55   346.63       1.2483     .9609      .2621
      2    .6240  .7320                          1.0351     .9700      .7379
  4   1    .4600  .3720    345.15   345.37       1.1793     .9605      .3521
      2    .5400  .6280                          1.0617     .9698      .6479
  5   1    .5400  .4620    344.05   344.31       1.1223     .9601      .4480
      2    .4600  .5380                          1.0976     .9697      .5520
  6   1    .6440  .5850    343.15   343.22       1.0652     .9598      .5814
      2    .3560  .4150                          1.1602     .9696      .4186
  7   1    .7250  .6920    342.55   342.60       1.0348     .9597      .6863
      2    .2750  .3080                          1.2201     .9697      .3137
  8   1    .8070  .7920    342.25   342.19       1.0151     .9599      .7885
      2    .1930  .2080                          1.2877     .9699      .2115
  9   1    .8380  .8280    342.15   342.09       1.0101     .9600      .8255
      2    .1620  .1720                          1.3145     .9700      .1745
 10   1    .8880  .8830    342.05   341.99       1.0045     .9605      .8823
      2    .1120  .1170                          1.3585     .9704      .1172
 11   1    .9500  .9470    341.95   342.00       1.0008     .9626      .9497
      2    .0500  .0530                          1.4136     .9720      .0503
 12   1    .9640  .9620    341.95   342.05       1.0004     .9641      .9641
      2    .0360  .0380                          1.4260     .9730      .0359

              ERROR ON X(1)= ABS(X(1)-XE(1))/DATA POINTS=    .0057

              ERROR ON T= ABS(TE-T)/DATA POINTS=   .10
-------------------------------------------------------------------------------
```

TABLE 4.12. DewT Results for n-Hexane(1)-Benzene(2) System Using UNIFAC(15)

```
PRESSURE=    1.000 ATM

                   GIVEN                                     CALCULATED
             -------------------    --------------------------------------------
DATA COMP    Y      XE       TE        T           GAMA       FHI         X
*******************************************************************************
  1   1    .1400  .0730    350.75   350.46       1.6076     .9622      .0680
      2    .8600  .9270                          1.0037     .9707      .9320
  2   1    .2680  .1720    348.25   347.98       1.4344     .9614      .1565
      2    .7320  .8280                          1.0185     .9702      .8435
  3   1    .3760  .2680    346.55   346.07       1.2933     .9607      .2572
      2    .6240  .7320                          1.0468     .9698      .7428
  4   1    .4600  .3720    345.15   344.77       1.1983     .9603      .3526
      2    .5400  .6280                          1.0828     .9696      .6474
  5   1    .5400  .4620    344.05   343.75       1.1265     .9599      .4533
      2    .4600  .5380                          1.1293     .9695      .5462
  6   1    .6440  .5850    343.15   342.77       1.0622     .9597      .5909
      2    .3560  .4150                          1.2044     .9695      .4091
  7   1    .7250  .6920    342.55   342.27       1.0315     .9596      .6953
      2    .2750  .3080                          1.2698     .9696      .3047
  8   1    .8070  .7920    342.25   341.98       1.0132     .9598      .7951
      2    .1930  .2080                          1.3382     .9698      .2049
  9   1    .8380  .8280    342.15   341.92       1.0087     .9600      .8309
      2    .1620  .1720                          1.3640     .9700      .1691
 10   1    .8880  .8830    342.05   341.88       1.0038     .9605      .8863
      2    .1120  .1170                          1.4053     .9704      .1137
 11   1    .9500  .9470    341.95   341.96       1.0007     .9626      .9510
      2    .0500  .0530                          1.4551     .9720      .0490
 12   1    .9640  .9620    341.95   342.02       1.0003     .9641      .9650
      2    .0360  .0380                          1.4661     .9730      .0350

              ERROR ON X(1)= ABS(X(1)-XE(1))/DATA POINTS=    .0070

              ERROR ON T= ABS(TE-T)/DATA POINTS=   .26
-------------------------------------------------------------------------------
```

TABLE 4.13. Bubble T Results for n-Hexane(1)-Toluene(2) System Using UNIQUAC(15)

```
PRESSURE=1. ATM
                      GIVEN.                                          CALCULATED
              ------------------    ------------------------------------------------
DATA COMP     X      YE      TE        T            GAMA        FHI        Y
************************************************************************************
  1    1    .1000  .3100   374.10    374.29       1.3130      .9681      .3098
       2    .9000  .6900                          1.0026      .9656      .6902
  2    1    .1960  .4840   367.55    367.53       1.2517      .9665      .4922
       2    .8040  .5160                          1.0103      .9639      .5078
  3    1    .2540  .5630   364.00    364.21       1.2189      .9657      .5718
       2    .7460  .4370                          1.0176      .9631      .4282
  4    1    .3520  .6640   359.50    359.52       1.1694      .9646      .6739
       2    .6480  .3360                          1.0352      .9619      .3261
  5    1    .3920  .6970   358.50    357.88       1.1511      .9641      .7074
       2    .6080  .3030                          1.0445      .9615      .2926
  6    1    .4430  .7420   355.65    355.96       1.1291      .9637      .7450
       2    .5570  .2580                          1.0584      .9610      .2550
  7    1    .5080  .7770   354.15    353.75       1.1035      .9632      .7865
       2    .4920  .2230                          1.0800      .9605      .2135
  8    1    .5790  .8220   351.65    351.61       1.0783      .9627      .8255
       2    .4210  .1780                          1.1093      .9600      .1745
  9    1    .6050  .8320   350.95    350.87       1.0699      .9625      .8385
       2    .3950  .1680                          1.1218      .9598      .1615
 10    1    .6400  .8480   349.90    349.93       1.0591      .9624      .8552
       2    .3600  .1520                          1.1403      .9596      .1448
 11    1    .7070  .8800   348.00    348.25       1.0407      .9621      .8848
       2    .2930  .1200                          1.1817      .9593      .1152
 12    1    .7300  .8900   347.35    347.70       1.0350      .9621      .8944
       2    .2700  .1100                          1.1980      .9592      .1056
 13    1    .7700  .9070   346.65    346.78       1.0261      .9620      .9107
       2    .2300  .0930                          1.2292      .9592      .0893
 14    1    .8130  .9270   345.40    345.84       1.0177      .9621      .9276
       2    .1870  .0730                          1.2675      .9592      .0724
 15    1    .8690  .9480   344.30    344.67       1.0091      .9627      .9492
       2    .1310  .0520                          1.3258      .9596      .0508

          ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=   .0055

          ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=   .23
------------------------------------------------------------------------------------
```

TABLE 4.14. Bubble T Results for n-Hexane(1)-Toluene(2) System Using UNIFAC(15)

```
PRESSURE=1.ATM
                      GIVEN                                           CALCULATED
              ------------------    ------------------------------------------------
DATA COMP     X      YE      TE        T            GAMA        FHI        Y
************************************************************************************
  1    1    .1000  .3100   374.10    373.60       1.3895      .9680      .3226
       2    .9000  .6900                          1.0041      .9654      .6774
  2    1    .1960  .4840   367.55    366.70       1.3037      .9663      .5022
       2    .8040  .5160                          1.0160      .9637      .4978
  3    1    .2540  .5630   364.00    363.42       1.2579      .9655      .5784
       2    .7460  .4370                          1.0271      .9629      .4216
  4    1    .3520  .6640   359.50    358.90       1.1906      .9644      .6750
       2    .6480  .3360                          1.0530      .9617      .3250
  5    1    .3920  .6970   358.50    357.33       1.1665      .9640      .7065
       2    .6080  .3030                          1.0663      .9613      .2935
  6    1    .4430  .7420   355.65    355.51       1.1384      .9635      .7422
       2    .5570  .2580                          1.0858      .9609      .2578
  7    1    .5080  .7770   354.15    353.43       1.1069      .9631      .7820
       2    .4920  .2230                          1.1147      .9604      .2180
  8    1    .5790  .8220   351.65    351.39       1.0775      .9626      .8201
       2    .4210  .1780                          1.1521      .9599      .1799
  9    1    .6050  .8320   350.95    350.70       1.0680      .9625      .8330
       2    .3950  .1680                          1.1674      .9597      .1670
 10    1    .6400  .8480   349.90    349.80       1.0563      .9623      .8496
       2    .3600  .1520                          1.1894      .9595      .1504
 11    1    .7070  .8800   348.00    348.17       1.0370      .9620      .8798
       2    .2930  .1200                          1.2366      .9592      .1202
 12    1    .7300  .8900   347.35    347.64       1.0314      .9620      .8897
       2    .2700  .1100                          1.2544      .9592      .1103
 13    1    .7700  .9070   346.65    346.74       1.0227      .9620      .9066
       2    .2300  .0930                          1.2874      .9591      .0934
 14    1    .8130  .9270   345.40    345.81       1.0150      .9621      .9244
       2    .1870  .0730                          1.3260      .9591      .0756
 15    1    .8690  .9480   344.30    344.64       1.0074      .9625      .9471
       2    .1310  .0520                          1.3815      .9595      .0529

          ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=   .0054

          ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=   .43
------------------------------------------------------------------------------------
```

TABLE 4.15. Bubble P Results for Benzene(1)-i-Propanol(2) System Using UNIQUAC(15)

```
     TEMPERATURE=  298.15 K

                     GIVEN                                            CALCULATED
              --------------------   ----------------------------------------
DATA COMP     X       YE        PE        P          GAMA        Y         FHI
*****************************************************************************
  1    1    .0760   .3650     .087      .086        3.1625     .3517     .9963
       2    .9240   .6350                           1.0057     .6483     .9940
  2    1    .1640   .5300     .111      .107        2.6908     .5184     .9953
       2    .8360   .4700                           1.0282     .4816     .9926
  3    1    .3000   .6350     .131      .127        2.1295     .6341     .9945
       2    .7000   .3650                           1.1039     .3659     .9913
  4    1    .4790   .7120     .139      .139        1.6227     .7039     .9939
       2    .5210   .2880                           1.3149     .2961     .9905
  5    1    .6380   .7450     .143      .143        1.3233     .7412     .9937
       2    .3620   .2550                           1.7063     .2588     .9902
  6    1    .8540   .7950     .143      .144        1.0705     .8003     .9937
       2    .1460   .2050                           3.2741     .1997     .9903
  7    1    .9410   .8700     .138      .139        1.0146     .8647     .9940
       2    .0590   .1300                           5.3074     .1353     .9907

            ERROR ON Y(1)= ABS(YE(1)-Y(1)/DATA POINTS=     .0069

            ERROR ON P= ABS(PE-P)/DATA POINTS=     .002
------------------------------------------------------------------------------
```

TABLE 4.16. Bubble P Results for Benzene(1)-i-Propanol(2) System Using UNIFAC(15)

```
     TEMPERATURE=  298.15 K

                     GIVEN                                            CALCULATED
              --------------------   ----------------------------------------
DATA COMP     X       YE        PE        P          GAMA        Y         FHI
*****************************************************************************
  1    1    .0760   .3650     .087      .086        3.1465     .3507     .9963
       2    .9240   .6350                           1.0053     .6493     .9940
  2    1    .1640   .5300     .111      .107        2.7087     .5206     .9953
       2    .8360   .4700                           1.0262     .4794     .9926
  3    1    .3000   .6350     .131      .128        2.1708     .6398     .9944
       2    .7000   .3650                           1.0977     .3602     .9912
  4    1    .4790   .7120     .139      .141        1.6582     .7098     .9938
       2    .5210   .2880                           1.3062     .2902     .9904
  5    1    .6380   .7450     .143      .145        1.3408     .7428     .9937
       2    .3620   .2550                           1.7146     .2572     .9901
  6    1    .8540   .7950     .143      .145        1.0700     .7929     .9937
       2    .1460   .2050                           3.4264     .2071     .9902
  7    1    .9410   .8700     .138      .140        1.0136     .8589     .9939
       2    .0590   .1300                           5.5650     .1411     .9906

            ERROR ON Y(1)= ABS(YE(1)-Y(1)/DATA POINTS=     .0066

            ERROR ON P= ABS(PE-P)/DATA POINTS=     .002
------------------------------------------------------------------------------
```

TABLE 4.17. Bubble T Results for Methanol(1)-2-Butanone(2) System Using UNIQUAC(15)

```
 PRESSURE=    1.000   ATM

                      GIVEN                                         CALCULATED
              --------------------     ----------------------------------------
DATA  COMP      X        YE        TE         T          GAMA        FHI        Y
*******************************************************************************
  1    1      .0760    .1930    348.45    343.96       3.0176      .9845      .2905
       2      .9240    .8070                           1.0130      .9663      .7095
  2    1      .1470    .3080    345.35    340.73       2.3763      .9836      .3923
       2      .8530    .6920                           1.0446      .9657      .6077
  3    1      .1970    .3770    343.85    339.45       2.0658      .9833      .4355
       2      .8030    .6230                           1.0759      .9654      .5645
  4    1      .2650    .4530    341.95    338.31       1.7620      .9830      .4783
       2      .7350    .5470                           1.1289      .9652      .5217
  5    1      .3560    .5280    340.65    337.33       1.4897      .9827      .5231
       2      .6440    .4720                           1.2175      .9651      .4769
  6    1      .4980    .6220    339.05    336.41       1.2375      .9823      .5868
       2      .5020    .3780                           1.3965      .9651      .4132
  7    1      .6220    .6950    338.25    336.01       1.1136      .9821      .6494
       2      .3780    .3050                           1.5957      .9653      .3506
  8    1      .7470    .7770    337.55    336.00       1.0429      .9820      .7300
       2      .2530    .2230                           1.8377      .9657      .2700
  9    1      .8290    .8320    337.45    336.25       1.0172      .9819      .7982
       2      .1710    .1680                           2.0156      .9662      .2018
 10    1      .8410    .8420    337.45    336.31       1.0146      .9819      .8095
       2      .1590    .1580                           2.0424      .9663      .1905
 11    1      .8730    .8690    337.45    336.49       1.0088      .9820      .8415
       2      .1270    .1310                           2.1146      .9666      .1585
 12    1      .9360    .9260    337.55    336.99       1.0019      .9821      .9134
       2      .0640    .0740                           2.2556      .9674      .0866

              ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=    .0420

              ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=  2.56
-------------------------------------------------------------------------------
```

TABLE 4.18. Bubble T Results for Methanol(1)-2-Butanone(2) System Using UNIFAC (15)

```
 PRESSURE=    1.000   ATM

                      GIVEN                                         CALCULATED
              --------------------     ----------------------------------------
DATA  COMP      X        YE        TE         T          GAMA        FHI        Y
*******************************************************************************
  1    1      .0760    .1930    348.45    348.31       1.7110      .9856      .1929
       2      .9240    .8070                           1.0032      .9673      .8071
  2    1      .1470    .3080    345.35    345.42       1.5975      .9846      .3139
       2      .8530    .6920                           1.0125      .9667      .6861
  3    1      .1970    .3770    343.85    343.88       1.5241      .9841      .3792
       2      .8030    .6230                           1.0229      .9665      .6208
  4    1      .2650    .4530    341.95    342.22       1.4334      .9836      .4513
       2      .7350    .5470                           1.0426      .9662      .5487
  5    1      .3560    .5280    340.65    340.58       1.3279      .9831      .5282
       2      .6440    .4720                           1.0800      .9661      .4718
  6    1      .4980    .6220    339.05    338.88       1.1966      .9326      .6242
       2      .5020    .3780                           1.1688      .9660      .3758
  7    1      .6220    .6950    338.25    337.94       1.1114      .9823      .6986
       2      .3780    .3050                           1.2853      .9661      .3014
  8    1      .7470    .7770    337.55    337.38       1.0505      .9821      .7762
       2      .2530    .2230                           1.4537      .9664      .2238
  9    1      .8290    .8320    337.45    337.23       1.0234      .9821      .8342
       2      .1710    .1680                           1.6023      .9667      .1658
 10    1      .8410    .8420    337.45    337.22       1.0203      .9821      .8435
       2      .1590    .1580                           1.6273      .9668      .1565
 11    1      .8730    .8690    337.45    337.23       1.0131      .9821      .8695
       2      .1270    .1310                           1.6983      .9670      .1305
 12    1      .9360    .9260    337.55    337.35       1.0034      .9822      .9277
       2      .0640    .0740                           1.8601      .9677      .0723

              ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=    .0019

              ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=   .17
-------------------------------------------------------------------------------
```

TABLE 4.19. Dew T Results for Ethanöl(1)-Water(2) System Using UNIQUAC(15)

```
    PRESSURE=   1.000 ATM

                       GIVEN                                     CALCULATED
              --------------------   -------------------------------------------
DATA  COMP     Y       XE       TE        T          GAMA        FHI          X
*********************************************************************************
  1    1     .1700   .0190   368.65   368.46       4.8592      .9829      .0189
       2     .8300   .9810                         1.0011      .9911      .9811
  2    1     .3891   .0721   362.15   361.41       3.6071      .9812      .0745
       2     .6109   .9279                         1.0163      .9909      .9255
  3    1     .4375   .0966   359.85   359.69       3.1849      .9809      .1010
       2     .5625   .9034                         1.0289      .9909      .8990
  4    1     .4704   .1238   358.45   358.51       2.8553      .9806      .1265
       2     .5296   .8762                         1.0437      .9909      .8735
  5    1     .5089   .1661   357.25   357.14       2.4227      .9803      .1697
       2     .4911   .8339                         1.0743      .9909      .8303
  6    1     .5445   .2337   355.85   355.92       2.0071      .9801      .2293
       2     .4555   .7663                         1.1264      .9909      .7707
  7    1     .5580   .2608   355.45   355.49       1.8570      .9800      .2582
       2     .4420   .7392                         1.1552      .9909      .7418
  8    1     .5826   .3273   354.65   354.75       1.6158      .9798      .3185
       2     .4174   .6727                         1.2226      .9910      .6815
  9    1     .6122   .3965   353.85   353.99       1.4056      .9797      .3959
       2     .3878   .6035                         1.3215      .9910      .6041
 10    1     .6564   .5079   352.95   353.10       1.2203      .9795      .5060
       2     .3436   .4921                         1.4841      .9911      .4940
 11    1     .6599   .5198   352.85   353.04       1.2088      .9795      .5146
       2     .3401   .4802                         1.4988      .9911      .4854
 12    1     .6841   .5732   352.45   352.67       1.1529      .9794      .5674
       2     .3159   .4268                         1.5853      .9912      .4326
 13    1     .7385   .6763   351.89   352.06       1.0754      .9794      .6721
       2     .2615   .3237                         1.7754      .9914      .3279
 14    1     .7815   .7472   351.56   351.75       1.0428      .9794      .7425
       2     .2185   .2528                         1.9129      .9916      .2575
 15    1     .8943   .8943   351.30   351.43       1.0064      .9801      .8920
       2     .1057   .1057                         2.2362      .9924      .1080

                    ERROR ON X(1)= ABS(X(1)-XE(1))/DATA POINTS=   .0036

                    ERROR ON T= ABS(TE-T)/DATA POINTS=   .18
---------------------------------------------------------------------------------
```

TAPLE 4.20. Dew T Results for Ethanol(1)-Water(2) System Using UNIFAC(15)

```
PRESSURE=1. ATM
                       GIVEN                                     CALCULATED
              --------------------   -------------------------------------------
DATA  COMP     Y       XE       TE        T          GAMA        FHI          X
*********************************************************************************
  1    1     .1700   .0190   368.65   368.37       5.9400      .9829      .0155
       2     .8300   .9810                         1.0010      .9911      .9845
  2    1     .3891   .0721   362.15   361.15       4.1199      .9812      .0659
       2     .6109   .9279                         1.0168      .9909      .9341
  3    1     .4375   .0966   359.85   359.40       3.5155      .9808      .0925
       2     .5625   .9034                         1.0310      .9909      .9075
  4    1     .4704   .1238   358.45   358.19       3.0337      .9806      .1204
       2     .5296   .8762                         1.0495      .9909      .8796
  5    1     .5089   .1661   357.25   356.81       2.4300      .9803      .1712
       2     .4911   .8339                         1.0901      .9909      .8288
  6    1     .5445   .2337   355.85   355.63       1.9223      .9800      .2421
       2     .4555   .7663                         1.1587      .9909      .7579
  7    1     .5580   .2608   355.45   355.21       1.7640      .9799      .2746
       2     .4420   .7392                         1.1941      .9909      .7254
  8    1     .5826   .3273   354.65   354.53       1.5466      .9798      .3355
       2     .4174   .6727                         1.2652      .9910      .6645
  9    1     .6122   .3965   353.85   353.82       1.3737      .9796      .4078
       2     .3878   .6035                         1.3571      .9910      .5922
 10    1     .6564   .5079   352.95   352.97       1.2213      .9795      .5081
       2     .3436   .4921                         1.4983      .9911      .4919
 11    1     .6599   .5198   352.85   352.91       1.2129      .9795      .5155
       2     .3401   .4802                         1.5092      .9911      .4845
 12    1     .6841   .5732   352.45   352.54       1.1625      .9794      .5654
       2     .3159   .4268                         1.5865      .9912      .4346
 13    1     .7385   .6763   351.89   351.91       1.0900      .9793      .6670
       2     .2615   .3237                         1.7588      .9914      .3330
 14    1     .7815   .7472   351.56   351.57       1.0555      .9794      .7385
       2     .2185   .2528                         1.8979      .9916      .2615
 15    1     .8943   .8943   351.30   351.25       1.0101      .9801      .8948
       2     .1057   .1057                         2.3128      .9924      .1052

                    ERROR ON X(1)= ABS(X(1)-XE(1))/DATA POINTS=   .0063

                    ERROR ON T= ABS(TE-T)/DATA POINTS=   .22
---------------------------------------------------------------------------------
```

TABLE 4.21. Bubble T Results for Methanol(1)-Water(2)
System Using UNIQUAC(15)

```
PRESSURE=   1.000  ATM

                     GIVEN                                       CALCULATED
             ------------------  ---------------------------------------
DATA COMP      X      YE       TE        T          GAMA      FHI       Y
*****************************************************************************
  1    1    .0293  .1831   368.40    368.18       2.2128    .9865    .1873
       2    .9707  .8169                          1.0010    .9911    .8127
  2    1    .0346  .2107   367.65    367.42       2.1886    .9864    .2136
       2    .9654  .7893                          1.0013    .9910    .7864
  3    1    .0406  .2363   366.85    366.60       2.1618    .9863    .2413
       2    .9594  .7637                          1.0018    .9910    .7587
  4    1    .0422  .2652   365.95    366.39       2.1547    .9862    .2483
       2    .9578  .7348                          1.0020    .9910    .7517
  5    1    .0577  .2978   364.95    364.49       2.0885    .9860    .3098
       2    .9423  .7022                          1.0037    .9909    .6902
  6    1    .0644  .3265   364.05    363.74       2.0610    .9859    .3331
       2    .9356  .6735                          1.0046    .9908    .6669
  7    1    .0737  .3608   363.15    362.76       2.0240    .9857    .3627
       2    .9263  .6392                          1.0060    .9908    .6373
  8    1    .0838  .3861   362.25    361.77       1.9852    .9856    .3918
       2    .9162  .6139                          1.0077    .9907    .6082
  9    1    .0948  .4142   362.35    360.78       1.9445    .9855    .4202
       2    .9052  .5858                          1.0098    .9907    .5798
 10    1    .2801  .6621   351.95    350.94       1.4578    .9842    .6661
       2    .7199  .3379                          1.0792    .9903    .3339
 11    1    .3004  .6882   350.75    350.29       1.4216    .9841    .6808
       2    .6996  .3118                          1.0904    .9903    .3192
 12    1    .3212  .6882   350.75    349.67       1.3871    .9840    .6947
       2    .6788  .3118                          1.1027    .9902    .3053
 13    1    .3435  .7002   350.05    349.04       1.3528    .9839    .7087
       2    .6565  .2998                          1.1167    .9902    .2913
 14    1    .3664  .7178   349.35    348.44       1.3202    .9839    .7220
       2    .6336  .2822                          1.1319    .9902    .2780
 15    1    .3909  .7274   348.85    347.84       1.2881    .9838    .7354
       2    .6091  .2726                          1.1491    .9902    .2646
 16    1    .4141  .7428   348.25    347.30       1.2601    .9837    .7475
       2    .5859  .2572                          1.1664    .9902    .2525
 17    1    .4391  .7597   347.75    346.74       1.2324    .9837    .7598
       2    .5609  .2403                          1.1860    .9902    .2402
 18    1    .4637  .7668   347.15    346.23       1.2073    .9836    .7714
       2    .5363  .2332                          1.2064    .9901    .2286
 19    1    .8457  .9360   340.35    339.88       1.0129    .9839    .9311
       2    .1543  .0640                          1.6634    .9905    .0689
 20    1    .8867  .9632   339.75    339.30       1.0068    .9844    .9487
       2    .1133  .0368                          1.7298    .9907    .0513
 21    1    .9293  .9771   338.85    338.73       1.0026    .9856    .9675
       2    .0707  .0229                          1.8029    .9914    .0325

            ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=    .0066

            ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=    .65
```

TABLE 4.22. Bubble T Results for Methanol(1)-Water(2) System Using UNIFAC(15)

```
 PRESSURE=    1.000  ATM

                         GIVEN                                           CALCULATED
                   ------------------         ------------------------------------------------
DATA  COMP     X      YE        TE         T            GAMA         FHI          Y
*********************************************************************************************
   1    1   .0293   .1831    368.40     368.38       2.1258       .9865       .1811
        2   .9707   .8169                            1.0011       .9911       .8189
   2    1   .0346   .2107    367.65     367.66       2.0979       .9864       .2063
        2   .9654   .7893                            1.0016       .9910       .7937
   3    1   .0406   .2363    366.85     366.89       2.0672       .9863       .2329
        2   .9594   .7637                            1.0021       .9910       .7671
   4    1   .0422   .2652    365.95     366.69       2.0592       .9863       .2396
        2   .9578   .7348                            1.0023       .9910       .7604
   5    1   .0577   .2978    364.95     364.91       1.9850       .9860       .2984
        2   .9423   .7022                            1.0042       .9909       .7016
   6    1   .0644   .3265    364.05     364.21       1.9547       .9859       .3207
        2   .9356   .6735                            1.0052       .9909       .6793
   7    1   .0737   .3608    363.15     363.30       1.9145       .9858       .3491
        2   .9263   .6392                            1.0068       .9908       .6509
   8    1   .0838   .3861    362.25     362.38       1.8729       .9857       .3770
        2   .9162   .6139                            1.0086       .9908       .6230
   9    1   .0948   .4142    362.35     361.46       1.8299       .9856       .4043
        2   .9052   .5858                            1.0109       .9907       .5957
  10    1   .2801   .6621    351.95     352.14       1.3633       .9843       .6496
        2   .7199   .3379                            1.0788       .9903       .3504
  11    1   .3004   .6882    350.75     351.49       1.3319       .9842       .6652
        2   .6996   .3118                            1.0891       .9903       .3348
  12    1   .3212   .6882    350.75     350.85       1.3023       .9842       .6803
        2   .6788   .3118                            1.1000       .9903       .3197
  13    1   .3435   .7002    350.05     350.21       1.2733       .9841       .6954
        2   .6565   .2998                            1.1123       .9903       .3046
  14    1   .3664   .7178    349.35     349.59       1.2461       .9840       .7101
        2   .6336   .2822                            1.1255       .9903       .2899
  15    1   .3909   .7274    348.85     348.96       1.2197       .9839       .7250
        2   .6091   .2726                            1.1401       .9902       .2750
  16    1   .4141   .7428    348.25     348.39       1.1969       .9839       .7384
        2   .5859   .2572                            1.1545       .9902       .2616
  17    1   .4391   .7597    347.75     347.80       1.1746       .9838       .7522
        2   .5609   .2403                            1.1706       .9902       .2478
  18    1   .4637   .7668    347.15     347.24       1.1547       .9838       .7653
        2   .5363   .2332                            1.1870       .9902       .2347
  19    1   .8457   .9360    340.35     340.15       1.0088       .9841       .9369
        2   .1543   .0640                            1.5043       .9906       .0631
  20    1   .8867   .9632    339.75     339.51       1.0046       .9847       .9538
        2   .1133   .0368                            1.5448       .9909       .0462
  21    1   .9293   .9771    338.85     338.87       1.0017       .9861       .9712
        2   .0707   .0229                            1.5882       .9916       .0288

            ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=    .0076

            ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=    .21
```

TABLE 4.23. Bubble T Results for Acetone(1)-Methanol(2)-Water(3) System Using UNIQUAC(16)

```
 PRESSURE=    1.000  ATM
                    GIVEN                                           CALCULATED
              --------------------   -----------------------------------------------------
DATA  COMP      X        YE        TE        T           GAMA         FHI         Y
*******************************************************************************************
  1     1     .2000    .6000     337.95    336.51       2.3595       .9743       .5911
        2     .2000    .2300                          1.2134       .9827       .2318
        3     .6000    .1700                          1.2780       .9911       .1770
  2     1     .2000    .4500     337.25    335.79       1.8879       .9747       .4622
        2     .4000    .4100                          1.0895       .9828       .4047
        3     .4000    .1400                          1.4892       .9909       .1331
  3     1     .2000    .3700     335.25    334.27       1.6405       .9758       .3822
        2     .6000    .5600                          1.0370       .9833       .5438
        3     .2000    .0700                          1.7750       .9911       .0740
  4     1     .4000    .6800     333.65    333.34       1.4767       .9740       .6690
        2     .2000    .1900                          1.1466       .9826       .1933
        3     .4000    .1300                          1.7238       .9914       .1377
  5     1     .4000    .5800     332.35    331.86       1.3223       .9752       .5701
        2     .4000    .3500                          1.1123       .9832       .3531
        3     .2000    .0700                          2.0602       .9915       .0768
  6     1     .6000    .7400     331.05    330.94       1.1434       .9746       .7213
        2     .2000    .1800                          1.2430       .9831       .1901
        3     .2000    .0800                          2.4804       .9919       .0886

              ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=      .0121

              ERROR ON Y(2)= ABS(Y(2)-YE(2))/DATA POINTS=      .0066

              ERROR ON Y(3)= ABS(Y(3)-YE(3))/DATA POINTS=      .0068

              ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=     .80
-------------------------------------------------------------------------------------------
```

TABLE 4.24. Bubble T Results for Acetone(1)-Methanol(2)-Water(3) System Using UNIFAC(16)

```
 PRESSURE=    1.000  ATM
                    GIVEN                                           CALCULATED
              --------------------   -----------------------------------------------------
DATA  COMP      X        YE        TE        T           GAMA         FHI         Y
*******************************************************************************************
  1     1     .2000    .6000     337.95    339.86       2.0370       .9748       .5662
        2     .2000    .2300                          1.0491       .9830       .2281
        3     .6000    .1700                          1.2789       .9911       .2057
  2     1     .2000    .4500     337.25    338.42       1.6212       .9751       .4309
        2     .4000    .4100                          1.0388       .9830       .4275
        3     .4000    .1400                          1.4070       .9909       .1416
  3     1     .2000    .3700     335.25    335.71       1.4723       .9764       .3589
        2     .6000    .5600                          1.0341       .9837       .5739
        3     .2000    .0700                          1.5073       .9912       .0671
  4     1     .4000    .6800     333.65    335.15       1.4252       .9743       .6841
        2     .2000    .1900                           .9682       .9829       .1753
        3     .4000    .1300                          1.6195       .9915       .1406
  5     1     .4000    .5800     332.35    333.11       1.2830       .9760       .5756
        2     .4000    .3500                          1.0730       .9838       .3580
        3     .2000    .0700                          1.6801       .9918       .0664
  6     1     .6000    .7400     331.05    331.68       1.1733       .9753       .7543
        2     .2000    .1800                          1.0722       .9836       .1689
        3     .2000    .0800                          2.0796       .9923       .0768

              ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=      .0144

              ERROR ON Y(2)= ABS(Y(2)-YE(2))/DATA POINTS=      .0112

              ERROR ON Y(3)= ABS(Y(3)-YE(3))/DATA POINTS=      .0096

              ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=     1.07
-------------------------------------------------------------------------------------------
```

TABLE 4.25. Dew T Results for 2-Butanone(1)-n-Heptane(2) -Toluene(3) System Using UNIQUAC(17)

```
   PRESSURE=    1.000 ATM

                       GIVEN                                         CALCULATED
              -------------------     -------------------------------------------------
DATA  COMP    Y       XE       TE        T            GAMA         FHI         X
***************************************************************************************
  1     1   .8380   .8560   351.15    351.72        1.0177       .9375       .8680
        2   .1570   .1270                           2.4245       .9808       .1212
        3   .0050   .0170                           1.2648       .9811       .0108
  2     1   .7630   .7380   351.15    351.35        1.0546       .9735       .7603
        2   .2190   .2170                           2.0470       .9592       .1982
        3   .0180   .0450                           1.1786       .9655       .0415
  3     1   .7620   .7430   351.15    351.17        1.0560       .9771       .7656
        2   .2270   .2250                           2.0377       .9646       .2088
        3   .0110   .0320                           1.1790       .9694       .0256
  4     1   .7160   .6580   351.00    351.16        1.1052       .9783       .6883
        2   .2740   .3140                           1.7907       .9662       .2874
        3   .0100   .0280                           1.1299       .9707       .0243
  5     1   .9250   .9350   352.05    352.73        1.0027       .9914       .9463
        2   .0710   .0430                           2.8221       .9872       .0459
        3   .0040   .0220                           1.3538       .9857       .0078
  6     1   .7510   .7040   351.97    352.07        1.0629       .9708       .7243
        2   .2120   .2060                           1.9945       .9552       .1916
        3   .0370   .0900                           1.1618       .9625       .0841
  7     1   .6850   .5880   351.97    351.72        1.1485       .9723       .6188
        2   .2900   .3460                           1.6530       .9570       .3204
        3   .0250   .0660                           1.1006       .9640       .0608
  8     1   .9860   .9720   352.85    353.29        1.0001       .9794       .9820
        2   .0060   .0040                           3.0611       .9693       .0034
        3   .0080   .0240                           1.4056       .9726       .0146
  9     1   .7320   .6580   353.15    353.23        1.0768       .9699       .6719
        2   .2030   .1960                           1.9197       .9538       .1833
        3   .0650   .1460                           1.1387       .9616       .1448
 10     1   .6450   .5140   353.07    352.84        1.2193       .9708       .5295
        2   .3100   .3790                           1.5018       .9545       .3626
        3   .0450   .1070                           1.0726       .9622       .1079
 11     1   .7000   .5780   355.40    355.27        1.1013       .9698       .5904
        2   .1860   .1730                           1.8201       .9536       .1659
        3   .1140   .2490                           1.1072       .9614       .2437
 12     1   .5790   .3940   355.33    355.03        1.3561       .9704       .3998
        2   .3420   .4310                           1.3300       .9537       .4208
        3   .0790   .1750                           1.0506       .9618       .1795
 13     1   .6610   .4990   357.65    357.45        1.1326       .9700       .5081
        2   .1720   .1540                           1.7258       .9539       .1511
        3   .1670   .3470                           1.0792       .9617       .3407
 14     1   .6540   .4820   358.05    357.96        1.1375       .9701       .4930
        2   .1660   .1490                           1.7152       .9540       .1445
        3   .1800   .3690                           1.0750       .9618       .3625
 15     1   .5870   .4030   358.00    357.70        1.2407       .9702       .4089
        2   .2530   .2630                           1.4810       .9538       .2570
        3   .1600   .3340                           1.0454       .9618       .3342
 16     1   .5040   .2820   358.00    357.63        1.5217       .9707       .2870
        2   .3810   .4770                           1.2144       .9539       .4731
        3   .1150   .2410                           1.0495       .9620       .2399
 17     1   .4440   .1910   358.00    357.84        1.9714       .9723       .1943
        2   .5060   .7050                           1.0722       .9557       .7034
        3   .0500   .1040                           1.1183       .9635       .0974
 18     1   .5250   .3180   360.30    359.91        1.3211       .9707       .3220
        2   .2710   .2770                           1.3813       .9543       .2757
        3   .2040   .4050                           1.0308       .9622       .4022
 19     1   .4350   .2080   360.27    360.04        1.6600       .9712       .2117
        2   .4180   .5060                           1.1542       .9544       .5071
        3   .1470   .2860                           1.0583       .9625       .2812
 20     1   .3920   .1480   360.30    360.13        1.9854       .9719       .1592
        2   .5160   .6750                           1.0697       .9550       .6740
        3   .0920   .1770                           1.1134       .9631       .1669
```

...Continued

TABLE 4.25 Continued.

```
21   1   .5640  .3500   362.65   362.49    1.2073   .9709   .3514
     2   .1400  .1130                      1.5835   .9552   .1150
     3   .2960  .5370                      1.0381   .9628   .5336
22   1   .4550  .2410   362.67   362.42    1.4062   .9712   .2440
     2   .2900  .2890                      1.3084   .9549   .2888
     3   .2550  .4700                      1.0237   .9628   .4672
23   1   .3350  .1180   362.77   362.60    1.9841   .9720   .1268
     2   .5220  .6340                      1.0708   .9552   .6320
     3   .1430  .2480                      1.1059   .9633   .2412
24   1   .5030  .2860   364.88   364.73    1.2576   .9714   .2825
     2   .1440  .1110                      1.5101   .9558   .1161
     3   .3530  .6030                      1.0239   .9633   .6014
25   1   .3880  .1830   364.90   364.70    1.4823   .9717   .1851
     2   .3110  .3010                      1.2591   .9555   .3009
     3   .3010  .5160                      1.0225   .9634   .5140
26   1   .2830  .0990   364.87   364.82    1.9652   .9724   .1016
     2   .5220  .5900                      1.0758   .9556   .5890
     3   .1950  .3110                      1.0965   .9637   .3094
27   1   .4060  .1980   368.25   368.20    1.3312   .9722   .1957
     2   .1490  .1120                      1.4322   .9567   .1145
     3   .4450  .6900                      1.0113   .9642   .6898
28   1   .3500  .1550   368.25   368.34    1.4177   .9724   .1578
     2   .2240  .1860                      1.3337   .9567   .1841
     3   .4260  .6590                      1.0105   .9642   .6580
29   1   .2840  .1090   368.20   368.07    1.5886   .9725   .1152
     2   .3450  .3160                      1.2074   .9564   .3157
     3   .3710  .5750                      1.0259   .9642   .5692
30   1   .1940  .0610   368.27   368.21    1.9726   .9731   .0632
     2   .5330  .5420                      1.0778   .9564   .5442
     3   .2730  .3970                      1.0900   .9644   .3926
31   1   .1970  .0730   373.30   373.24    1.5212   .9735   .0726
     2   .2470  .1840                      1.2773   .9580   .1848
     3   .5560  .7430                      1.0095   .9654   .7426
32   1   .1240  .0380   373.05   372.88    1.7199   .9737   .0408
     2   .3990  .3330                      1.1619   .9577   .3314
     3   .4770  .6290                      1.0354   .9654   .6278

               ERROR ON X(1)= ABS(X(1)-XE(1))/DATA POINTS=    .0093

               ERROR ON X(2)= ABS(X(2)-XE(2))/DATA POINTS=    .0063

               ERROR ON X(3)= ABS(X(3)-XE(3))/DATA POINTS=    .0042

               ERROR ON T= ABS(TE-T)/DATA POINTS=    .21
```

TABLE 4.26. Dew T Results for 2-Butanone(1)-n-Heptane(2) -Toluene(3) System Using UNIFAC(17)

```
PRESSURE=   1.000 ATM
                     GIVEN                               CALCULATED
             ---------------------    ----------------------------------------
DATA COMP    Y      XE       TE        T          GAMA       FHI        X
**************************************************************************
  1    1   .8380  .8560   351.15    351.22      1.0187     .9875     .8805
       2   .1570  .1270                         2.8078     .9807     .1064
       3   .0050  .0170                         1.0565     .9811     .0131
  2    1   .7630  .7380   351.15    350.89      1.0649     .9734     .7638
       2   .2190  .2170                         2.2318     .9591     .1846
       3   .0180  .0450                          .9606     .9654     .0517
  3    1   .7620  .7430   351.15    350.55      1.0640     .9770     .7744
       2   .2270  .2250                         2.2485     .9644     .1931
       3   .0110  .0320                          .9478     .9693     .0325
  4    1   .7160  .6580   351.00    350.41      1.1216     .9782     .6941
       2   .2740  .3140                         1.9242     .9660     .2740
       3   .0100  .0280                          .8831     .9705     .0319
  5    1   .9250  .9350   352.05    352.52      1.0029     .9914     .9521
       2   .0710  .0430                         3.3508     .9871     .0389
       3   .0040  .0220                         1.1835     .9857     .0090
  6    1   .7510  .7040   351.97    351.94      1.0782     .9708     .7169
       2   .2120  .2060                         2.1075     .9551     .1821
       3   .0370  .0900                          .9719     .9625     .1010
  7    1   .6850  .5880   351.97    351.30      1.1762     .9722     .6122
       2   .2900  .3460                         1.7253     .9568     .3112
       3   .0250  .0660                          .8862     .9638     .0766
  8    1   .9860  .9720   352.85    353.33      1.0002     .9794     .9809
       2   .0060  .0040                         3.6390     .9693     .0029
       3   .0080  .0240                         1.2631     .9726     .0162
  9    1   .7320  .6580   353.15    353.47      1.0935     .9700     .6568
       2   .2030  .1960                         1.9711     .9539     .1772
       3   .0650  .1460                          .9843     .9616     .1661
 10    1   .6450  .5140   353.07    352.77      1.2477     .9708     .5185
       2   .3100  .3790                         1.5466     .9545     .3529
       3   .0450  .1070                          .9016     .9622     .1286
 11    1   .7000  .5780   355.40    355.96      1.1091     .9699     .5744
       2   .1860  .1730                         1.8262     .9538     .1618
       3   .1140  .2490                          .9998     .9616     .2638
 12    1   .5790  .3940   355.33    355.33      1.3478     .9705     .3986
       2   .3420  .4310                         1.3778     .9538     .4024
       3   .0790  .1750                          .9379     .9618     .1990
 13    1   .6610  .4990   357.65    358.40      1.1222     .9702     .4987
       2   .1720  .1540                         1.7197     .9542     .1473
       3   .1670  .3470                         1.0070     .9620     .3540
 14    1   .6540  .4820   358.05    358.95      1.1225     .9703     .4853
       2   .1660  .1490                         1.7073     .9544     .1408
       3   .1800  .3690                         1.0091     .9621     .3739
 15    1   .5870  .4030   358.00    358.56      1.2066     .9704     .4100
       2   .2530  .2630                         1.5150     .9541     .2446
       3   .1600  .3340                          .9835     .9620     .3454
 16    1   .5040  .2820   358.00    358.04      1.4425     .9708     .2991
       2   .3810  .4770                         1.2699     .9541     .4467
       3   .1150  .2410                          .9771     .9622     .2542
 17    1   .4440  .1910   358.00    357.67      1.9725     .9722     .1951
       2   .5060  .7050                         1.0931     .9557     .6984
       3   .0500  .1040                         1.0287     .9635     .1064
 18    1   .5250  .3180   360.30    360.79      1.2422     .9709     .3339
       2   .2710  .2770                         1.4275     .9546     .2599
       3   .2040  .4050                          .9923     .9625     .4062
 19    1   .4350  .2080   360.27    360.40      1.5175     .9713     .2291
       2   .4180  .5060                         1.2065     .9545     .4798
       3   .1470  .2860                         1.0103     .9626     .2911
 20    1   .3920  .1480   360.30    360.12      1.8787     .9719     .1682
       2   .5160  .6750                         1.0993     .9550     .6560
       3   .0920  .1770                         1.0574     .9631     .1757
```

···Continued.

TABLE 4.26. Continued.

21	1	.5640	.3500	362.65	363.60	1.1425	.9712	.3599
	2	.1400	.1130			1.5872	.9556	.1110
	3	.2960	.5370			1.0108	.9631	.5291
22	1	.4550	.2410	362.67	363.21	1.2738	.9714	.2633
	2	.2900	.2890			1.3615	.9552	.2711
	3	.2550	.4700			1.0020	.9630	.4655
23	1	.3350	.1180	362.77	362.65	1.7917	.9721	.1402
	2	.5220	.6340			1.1039	.9552	.6122
	3	.1430	.2480			1.0757	.9633	.2476
24	1	.5030	.2860	364.88	365.77	1.1612	.9717	.2972
	2	.1440	.1110			1.5292	.9561	.1112
	3	.3530	.6030			1.0080	.9636	.5915
25	1	.3880	.1830	364.90	365.34	1.3018	.9719	.2070
	2	.3110	.3010			1.3141	.9557	.2830
	3	.3010	.5160			1.0104	.9635	.5100
26	1	.2830	.0990	364.87	364.85	1.7140	.9724	.1163
	2	.5220	.5900			1.1099	.9556	.5704
	3	.1950	.3110			1.0822	.9637	.3132
27	1	.4060	.1980	368.25	369.04	1.1859	.9724	.2147
	2	.1490	.1120			1.4698	.9570	.1090
	3	.4450	.6900			1.0054	.9644	.6763
28	1	.3500	.1550	368.25	368.99	1.2322	.9725	.1784
	2	.2240	.1860			1.3847	.9569	.1741
	3	.4260	.6590			1.0068	.9644	.6475
29	1	.2840	.1090	368.20	368.41	1.3388	.9726	.1354
	2	.3450	.3160			1.2615	.9565	.2992
	3	.3710	.5750			1.0222	.9643	.5654
30	1	.1940	.0610	368.27	368.08	1.6554	.9730	.0755
	2	.5330	.5420			1.1035	.9564	.5310
	3	.2730	.3970			1.0918	.9644	.3935
31	1	.1970	.0730	373.30	373.46	1.2635	.9735	.0869
	2	.2470	.1840			1.3355	.9580	.1757
	3	.5560	.7430			1.0101	.9654	.7374
32	1	.1240	.0380	373.05	372.72	1.3853	.9737	.0509
	2	.3990	.3330			1.2078	.9577	.3201
	3	.4770	.6290			1.0383	.9653	.6290

```
ERROR ON X(1)= ABS(X(1)-XE(1))/DATA POINTS=    .0156

ERROR ON X(2)= ABS(X(2)-XE(2))/DATA POINTS=    .0172

ERROR ON X(3)= ABS(X(3)-XE(3))/DATA POINTS=    .0082

ERROR ON T= ABS(TE-T)/DATA POINTS=    .41
```

TABLE 4.27. Bubble P Results for Methnol(1)-Carbontetrachloride(2)-Benzene(3) System Using UNIQUAC(18)

```
     TEMPERATURE=  328.15 K

                          GIVEN                                        CALCULATED
                 --------------------    ---------------------------------------------
DATA COMP    X       YE        PE          P             GAMA          Y         FHI
***************************************************************************************
 1    1    .1880   .5152      .875        .887         3.6159        .5228      .9831
      2    .1960   .1387                               1.2361        .1362      .9690
      3    .6160   .3461                               1.1210        .3409      .9698
 2    1    .1983   .5130      .908        .920         3.5335        .5197      .9826
      2    .3961   .2624                               1.2013        .2582      .9679
      3    .4056   .2246                               1.1495        .2221      .9688
 3    1    .1982   .5109      .907        .920         3.5350        .5197      .9826
      2    .3963   .2628                               1.2012        .2583      .9679
      3    .4055   .2263                               1.1494        .2221      .9688
 4    1    .1945   .5068      .930        .943         3.6717        .5171      .9824
      2    .5922   .3733                               1.1682        .3665      .9674
      3    .2133   .1199                               1.1728        .1164      .9683
 5    1    .3590   .5397      .936        .950         2.1228        .5475      .9820
      2    .3230   .2539                               1.4695        .2495      .9669
      3    .3180   .2064                               1.3826        .2030      .9678
 6    1    .5557   .5672      .944        .958         1.4439        .5719      .9818
      2    .2134   .2316                               2.0582        .2291      .9667
      3    .2309   .2012                               1.3826        .1991      .9677
 7    1    .7515   .6209      .925        .942         1.1349        .6179      .9820
      2    .1115   .1925                               3.3169        .1960      .9674
      3    .1370   .1866                               2.9207        .1862      .9683
 8    1    .8433   .6736      .896        .915         1.0562        .6641      .9825
      2    .0814   .1890                               4.4463        .1972      .9686
      3    .0753   .1374                               3.8486        .1387      .9695

           ERROR ON Y(1)= ABS(YE(1)-Y(1)/DATA POINTS=    .0073

           ERROR ON Y(2)= ABS(YE(2)-Y(2)/DATA POINTS=    .0046

           ERROR ON Y(3)= ABS(YE(3)-Y(3)/DATA POINTS=    .0028

           ERROR ON P= ABS(PE-P)/DATA POINTS=     .014
---------------------------------------------------------------------------------------
```

TABLE 4.28 Bubble P Results for Methanol(1)-Carbontetrachloride(2)-Benzene(3) System Using UNIFAC(18)

```
     TEMPERATURE=  328.15 K

                          GIVEN                                        CALCULATED
                 --------------------    ---------------------------------------------
DATA COMP    X       YE        PE          P             GAMA          Y         FHI
***************************************************************************************
 1    1    .1880   .5152      .875        .575         2.1927        .4857      .9891
      2    .1960   .1387                                .8258        .1387      .9798
      3    .6160   .3461                                .8100        .3756      .9803
 2    1    .1983   .5130      .908        .720         2.9049        .5440      .9864
      2    .3961   .2624                               1.1136        .3037      .9750
      3    .4056   .2246                                .6212        .1523      .9757
 3    1    .1982   .5109      .907        .720         2.9068        .5440      .9864
      2    .3963   .2628                               1.1135        .3038      .9750
      3    .4055   .2263                                .6211        .1522      .9757
 4    1    .1945   .5068      .930        .863         3.5337        .5426      .9842
      2    .5922   .3733                               1.1798        .4029      .9709
      3    .2133   .1199                                .5038        .0544      .9717
 5    1    .3590   .5397      .936        .751         1.6788        .5457      .9859
      2    .3230   .2539                               1.5473        .3301      .9740
      3    .3180   .2064                                .6733        .1242      .9748
 6    1    .5557   .5672      .944        .781         1.2075        .5845      .9853
      2    .2134   .2316                               2.3334        .3164      .9732
      3    .2309   .2012                                .7691        .0991      .9739
 7    1    .7515   .6209      .925        .783         1.0471        .6838      .9853
      2    .1115   .1925                               3.5307        .2494      .9737
      3    .1370   .1866                                .8758        .0668      .9744
 8    1    .8433   .6736      .896        .786         1.0197        .7446      .9855
      2    .0814   .1890                               4.2372        .2177      .9744
      3    .0753   .1374                                .9050        .0378      .9750

           ERROR ON Y(1)= ABS(YE(1)-Y(1)/DATA POINTS=    .0358

           ERROR ON Y(2)= ABS(YE(2)-Y(2)/DATA POINTS=    .0448

           ERROR ON Y(3)= ABS(YE(3)-Y(3)/DATA POINTS=    .0806

           ERROR ON P= ABS(PE-P)/DATA POINTS=     .167
---------------------------------------------------------------------------------------
```

TABLE 4.29. Dew P Results for Methanol(1)-Carbontetrachloride(2)-Benzene(3) System Using UNIQUAC(18)

```
TEMPERATURE= 328.15 K

                    GIVEN                                       CALCULATED
             --------------------       --------------------------------------
DATA  COMP      Y       XE        PE        P          GAMA        FHI        X
**********************************************************************************
  1     1    .5152    .1880     .875      .877        3.9207      .9833     .1691
        2    .1387    .1960                           1.2125      .9693     .2014
        3    .3461    .6160                           1.1020      .9701     .6296
  2     1    .5130    .1983     .908      .911        3.8485      .9828     .1781
        2    .2624    .3961                           1.1759      .9682     .4078
        3    .2246    .4056                           1.1287      .9691     .4141
  3     1    .5109    .1982     .907      .909        3.9588      .9828     .1719
        2    .2628    .3963                           1.1685      .9683     .4097
        3    .2263    .4055                           1.1223      .9691     .4183
  4     1    .5068    .1945     .930      .929        4.2650      .9827     .1618
        2    .3733    .5922                           1.1294      .9678     .6152
        3    .1199    .2133                           1.1396      .9687     .2230
  5     1    .5397    .3590     .936      .944        2.4646      .9821     .3027
        2    .2539    .3230                           1.3605      .9671     .3526
        3    .2064    .3180                           1.2886      .9681     .3447
  6     1    .5672    .5557     .944      .957        1.5173      .9818     .5242
        2    .2316    .2134                           1.9373      .9667     .2291
        3    .2012    .2309                           1.7798      .9677     .2467
  7     1    .6209    .7515     .925      .940        1.1285      .9820     .7579
        2    .1925    .1115                           3.3788      .9675     .1073
        3    .1866    .1370                           2.9694      .9684     .1348
  8     1    .6736    .8433     .896      .908        1.0490      .9826     .8543
        2    .1890    .0814                           4.6303      .9689     .0743
        3    .1374    .0753                           3.9912      .9698     .0714

          ERROR ON X(1)= ABS(XE(1)-X(1))/DATA POINTS=    .0254

          ERROR ON X(2)= ABS(XE(2)-X(2))/DATA POINTS=    .0137

          ERROR ON X(3)= ABS(XE(3)-X(3))/DATA POINTS=    .0117

          ERROR ON PRESSURE= ABS(PE-P)/DATA POINTS=   .007
----------------------------------------------------------------------------------
```

TABLE 4.30. Dew P Results for Methanol(1)-Carbontetrarachloride(2)-Benzene(3) System Using UNIFAC(18)

```
TEMPERATURE= 328.15 K

                    GIVEN                                       CALCULATED
             --------------------       ----------------------------------------
DATA  COMP      Y       XE        PE        P          GAMA        FHI        X
************************************************************************************
  1     1    .5152    .1880     .875      .893        4.7821      .9830     .1412
        2    .1387    .1960                           1.2196      .9687     .2038
        3    .3461    .6160                           1.0784      .9696     .6550
  2     1    .5130    .1983     .908      .934        4.9073      .9824     .1430
        2    .2624    .3961                           1.1610      .9674     .4227
        3    .2246    .4056                           1.1016      .9683     .4343
  3     1    .5109    .1982     .907      .930        5.0946      .9824     .1368
        2    .2628    .3963                           1.1533      .9675     .4247
        3    .2263    .4055                           1.0955      .9684     .4385
  4     1    .5068    .1945     .930      .952        6.3555      .9822     .1112
        2    .3733    .5922                           1.0879      .9670     .6540
        3    .1199    .2133                           1.1085      .9680     .2348
  5     1    .5397    .3590     .936      .956        1.3775      .9819     .5487
        2    .2539    .3230                           2.1484      .9667     .2261
        3    .2064    .3180                           1.9977      .9676     .2252
  6     1    .5672    .5557     .944      .948        1.1850      .9820     .6648
        2    .2316    .2134                           2.6946      .9671     .1632
        3    .2012    .2309                           2.5275      .9680     .1721
  7     1    .6209    .7515     .925      .918        1.0770      .9825     .7760
        2    .1925    .1115                           3.4139      .9683     .1038
        3    .1866    .1370                           3.2548      .9691     .1202
  8     1    .6736    .8433     .896      .885        1.0357      .9831     .8442
        2    .1890    .0814                           3.9871      .9697     .0842
        3    .1374    .0753                           3.3875      .9705     .0715

          ERROR ON X(1)= ABS(XE(1)-X(1))/DATA POINTS=    .0714

          ERROR ON X(2)= ABS(XE(2)-X(2))/DATA POINTS=    .0353

          ERROR ON X(3)= ABS(XE(3)-X(3))/DATA POINTS=    .0368

          ERROR ON PRESSURE= ABS(PE-P)/DATA POINTS=   .016
------------------------------------------------------------------------------------
```

TABLE 4.31. VLE Results for Various Alcohol-Aromatic Binary Sysems (15)

SYSTEM		TYPE	T(P) K(ATM)	DATA POINTS	AMD(UNIQUAC)		AMD(UNIFAC)		AMD(RAOULT)	
					X(Y)	T(P)	X(Y)	T(P)	X(Y)	T(P)
METHANOL	TOLUENE	BUBT	1.000	10	.0104	.77	.0049	.24	.1047	9.88
BENZENE	N-BUTANOL	BUBT	1.000	21	.0290	.23	.0047	.34	.0790	6.29
METHANOL	BENZENE	BUBT	1.000	10	.0083	.55	.0156	.76	.1871	10.47
BENZENE	N-PROPANOL	BUBT	1.000	12	.0422	1.21	.0131	1.36	.0926	7.65
ETHANOL	BENZENE	BUBT	1.000	10	.0083	.32	.0067	.49	.1399	9.19
METHANOL	TOLUENE	DEWT	1.000	10	.0430	.55	.0242	.19	.1919	11.28
METHANOL	BENZENE	DEWT	1.000	10	.0140	.29	.0233	.25	.1800	9.81
BENZENE	N-BUTANOL	DEWT	1.000	21	.0338	1.28	.0097	.35	.0852	5.18
ETHANOL	BENZENE	DEWT	1.000	10	.0271	.37	.0195	.47	.1407	9.22
BENZENE	N-BUTANOL	BUBP	293.15	5	.0143	.002	.0138	.002	.1492	.030
BENZENE	N-BUTANOL	BUBP	318.15	9	.0041	.001	.0039	.005	.0429	.058
BENZENE	SEC-BUTANOL	BUBP	298.15	5	.0667	.024	.0123	.002	.0715	.033
BENZENE	TER-BUTANOL	BUBP	298.15	6	.0777	.022	.0171	.001	.0891	.034
METHANOL	BENZENE	BUBP	328.15	9	.0089	.012	.0118	.012	.1693	.279
ETHANOL	BENZENE	BUBP	323.15	11	.0173	.009	.0088	.004	.1474	.127
ETHANOL	TOLUENE	BUBP	308.15	10	.0297	.005	.0198	.003	.1826	.047
ETHANOL	TOLUENE	BUBP	358.15	11	.0171	.037	.0204	.044	.1211	.358
BENZENE	I-PROPANOL	BUBP	298.15	7	.0069	.002	.0066	.002	.1346	.036
BENZENE	N-BUTANOL	DEWP	298.15	5	.1492	.014	.1463	.014	.3892	.074
BENZENE	N-BUTANOL	DEWP	318.15	9	.0232	.005	.0250	.009	.4970	.203
BENZENE	SEC-BUTANOL	DEWP	298.15	5	.1171	.019	.0700	.006	.3723	.078
BENZENE	TER-BUTANOL	DEWP	298.15	6	.1014	.019	.0380	.002	.4361	.095
BENZENE	I-PROPANOL	DEWP	298.15	7	.0127	.001	.0088	.002	.4007	.098
METHANOL	BENZENE	DEWP	328.15	9	.0211	.008	.0419	.009	.3826	.657
ETHANOL	BENZENE	DEWP	323.15	11	.0244	.005	.0117	.003	.5305	.436
BENZENE	N-PROPANOL	DEWP	313.15	10	.0352	.009	.0365	.008	.3848	.175

AMD=AVERAGE ABSOLUTE MEAN DEVIATION

TABLE 4.32 VLE Results for various Alkane- Aromatic Binary Systems (15)

SYSTEM		TYPE	T(P) K(ATM)	DATA POINTS	AMD(UNIQUAC)		AMD(UNIFAC)		AMD(RAOULT)	
					X(Y)	T(P)	X(Y)	T(P)	X(Y)	T(P)
N-HEXANE	BENZENE	DEWT	1.000	12	.0057	.10	.0070	.26	.0279	2.19
N-HEXANE	TOLUENE	BUBT	1.000	15	.0055	.23	.0054	.43	.0181	2.37
BENZENE	N-HEPTANE	BUBT	1.000	18	.0080	.50	.0058	.34	.0227	2.27
N-HEPTANE	TOLUENE	BUBT	1.000	17	.0025	.16	.0070	.50	.0167	1.46
224 T.M.P.	TOLUENE	BUBP	373.15	9	.0136	.224	.0040	.015	.0264	.053
BENZENE	N-HEPTANE	DEWT	1.000	18	.0083	.42	.0060	.27	.2460	2.26
N-HEPTANE	TOLUENE	DEWT	1.000	17	.0024	.14	.0067	.44	.0167	1.46
224 T.M.P.	TOLUENE	DEWP	373.15	9	.0140	.021	.0130	.010	.0266	.054

T.M.P= TRIMETHYL PENTANE

TABLE 4.33. VLE Results for various Alkane-Alcohol Binary Systems (15)

			T(P)	DATA	AMD(UNIQUAC)		AMD(UNIFAC)		AMD(RAOULT)	
SYSTEM		TYPE	K(ATM)	POINTS	X(Y)	T(P)	X(Y)	T(P)	X(Y)	T(P)
N-HEXANE	ETHANOL	BUBT	1.000	9	.0046	.45	.0151	.46	.1878	13.92
N-DECANE	N-BUTANOL	BUBP	373.15	19	.0134	.004	.0116	.013	.0301	.094
N-DECANE	N-BUTANOL	DEWP	373.15	19	.0449	.008	.0415	.014	.1500	.118
N-HEPTANE	N-BUTANOL	BUBT	.900	10	.0312	2.09	.0303	1.53	.1479	11.70
ETHANOL	N-HEPTANE	BUBP	323.15	12	.0306	.010	.0256	.010	.1322	.136
METHANOL	N-HEPTANE	BUBT	1.000	7	.0109	.55	.0229	.83	.2047	15.91
N-PROPANOL	N-HEPTANE	BUBT	1.000	9	.0316	1.64	.0292	1.08	.1374	11.48
N-HEXANE	N-PROPANOL	BUBT	1.000	12	.0392	1.72	.0452	1.65	.1465	11.12
METHANOL	N-HEXANE	BUBP	318.15	9	.0150	.020	.0208	.034	.2177	.379
I-PROPANOL	224 T.M.P.	BUBT	1.000	12	.0067	.35	.0485	3.63	.1248	8.65
N-HEPTANE	N-BUTANOL	DEWT	.900	10	.0505	1.15	.0556	.71	.1436	10.22
ETHANOL	N-HEPTANE	DEWP	323.15	12	.0766	.010	.0632	.010	.1933	.143
METHANOL	N-HEPTANE	DEWT	1.000	7	.0836	.14	.2276	.39	.2769	16.35
N-PROPANOL	N-HEPTANE	DEWT	1.000	9	.0656	.83	.0678	.83	.1376	11.48
N-HEXANE	N-PROPANOL	DEWT	1.000	12	.0382	2.11	.0538	1.48	.1406	8.96
METHANOL	N-HEXANE	DEWP	318.15	9	.3134	.008	.1635	.002	.2177	.379
I-PROPANOL	224 T.M.P.	DEWT	1.000	12	.0139	.35	.0649	2.08	.1265	8.37

T.M.P=TRIMETHYL PENTANE

TABLE 4.34 VLE Results for Alcohol-Water Binary Systems (15)

			T(P)	DATA	AMD(UNIQUAC)		AMD(UNIFAC)		AMD(RAOULT)	
SYSTEM		TYPE	K(ATM)	POINTS	X(Y)	T(P)	X(Y)	T(P)	X(Y)	T(P)
N-BUTANOL	WATER	BUBT	1.000	13	.0419	1.51	.0507	1.76	.1875	10.35
N-PROPANOL	WATER	BUBT	1.000	3	.0079	.21	.0142	.46	.1351	11.10
METHANOL	WATER	BUBT	1.000	51	.0114	.70	.0130	.33	.0832	4.62
ETHANOL	WATER	BUBT	1.000	15	.0027	.14	.0058	.31	.1179	7.45
ETHANOL	WATER	DEWT	1.000	15	.0036	.18	.0063	.22	.1012	6.41

TABLE 4.35. VLE Results for Ketone-Alcohol Binary Systems (15)

			T(P)	DATA	AMD(UNIQUAC)		AMD(UNIFAC)		AMD(RAOULT)	
SYSTEM		TYPE	K(ATM)	POINTS	X(Y)	T(P)	X(Y)	T(P)	X(Y)	T(P)
ACETONE	ETHANOL	BUBT	1.000	9	.0220	.41	.0265	.69	.0459	3.42
ACETONE	ETHANOL	DEWT	1.000	9	.0226	.32	.0264	.11	.0410	3.29
ACETONE	METHANOL	BUBT	1.000	8	.0169	.51	.0136	.36	.0424	2.70
ACETONE	METHANOL	DEWT	1.000	8	.0173	.46	.0140	.36	.0432	2.66
METHANOL	2-BUTANONE	BUBT	1.000	12	.0420	2.56	.0019	.17	.0527	3.28
METHANOL	2-BUTANONE	DEWT	1.000	12	.0437	1.85	.0021	.18	.0565	3.27

TABLE 4.36. VLE Results for Ternary Systems

		T(P)	DATA	AMD(UNIQUAC)		AMD(UNIFAC)		AMD(RAOULT)	
SYSTEM	TYPE	K(ATM)	POINTS	X(Y)	T(P)	X(Y)	T(P)	X(Y)	T(P)
ACETONE	BUBT	1.000	6	.0121	.80	.0144	1.07	.0561	7.92
METHANOL				.0066		.0112		.0772	
WATER(16)				.0068		.0096		.0290	
ACETONE	DEWT	1.000	6	.0263	1.00	.0235	.75	.0650	7.89
METHANOL				.0081		.0160		.0650	
WATER(16)				.0266		.0293		.0619	
2-BUTANONE	BUBT	1.000	32	.0069	.18	.0172	.68	.0583	6.47
N-HEPTANE				.0047		.0144		.0487	
TOLUENE(17)				.0028		.0075		.0294	
2-BUTANONE	DEWT	1.000	32	.0093	.21	.0156	.41	.0529	5.38
N-HEPTANE				.0063		.0172		.0537	
TOLUENE(17)				.0042		.0082		.0341	
METHANOL	DEWP	328.15	8	.0254	.007	.0714	.016	.3232	.729
CCL4				.0137		.0353		.2061	
BENZENE(18)				.0117		.0368		.1919	
METHANOL	BUBP	328.15	8	.0073	.142	.0358	.168	.1967	.365
CCL4				.0046		.0448		.1025	
BENZENE(18)				.0028		.0806		.0942	
METHANOL	DEWP	307.83	6	.0404	.004	.0968	.004	.2798	.303
CCL4				.0206		.0463		.2003	
BENZENE(18)				.0206		.0505		.1846	
METHANOL	BUBP	307.83	6	.0071	.001	.0157	.008	.1771	.165
CCL4				.0045		.0058		.0921	
BENZENE(18)				.0047		.0099		.0850	
WATER	BUBT	1.000	67	.0394	3.93	.0445	6.29	.0196	2.23
FORMIC ACID				.0135		.0291		.0375	
ACETIC ACID(19)				.0271		.0384		.0383	
WATER	DEWT	1.000	67	.0430	3.46	.0555	5.52	.0239	1.72
FORMIC ACID				.0127		.0316		.0366	
ACETIC ACID(19)				.0346		.0535		.0491	

TABLE 4.37. VLE Results for Ethanol-Water Systems at Different Conditions(15)

	T(P)	DATA	AMD(UNIQUAC)		AMD(UNIFAC)		AMD(RAOULT)	
TYPE	K(ATM)	POINTS	X(Y)	T(P)	X(Y)	T(P)	X(T)	T(P)
DEWT	.066	11	.0141	.43	.0214	.54	.0898	4.37
DEWT	.329	11	.0176	.23	.0219	.25	.0967	4.85
DEWT	.658	11	.0068	.12	.0102	.12	.0982	5.60
DEWT	.929	12	.0029	.15	.0052	.27	.0927	5.04
DEWT	1.000	15	.0036	.18	.0063	.22	.1012	6.41
DEWT	3.402	18	.0061	.33	.0097	.32	.0961	6.76
DEWT	6.805	18	.0407	.64	.0464	1.14	.1024	6.44
DEWT	13.610	18	.0231	1.32	.0302	2.07	.0799	6.96
DEWT	20.410	12	.0313	1.01	.0421	1.82	.0682	7.66
BUBT	.066	11	.0179	.58	.0214	.81	.0766	4.01
BUBT	.329	11	.0112	.36	.0150	.53	.0983	5.25
BUBT	.658	11	.0045	.13	.0070	.24	.1005	5.99
BUBT	.929	12	.0047	.17	.0096	.53	.1426	7.36
BUBT	1.000	15	.0027	.14	.0058	.31	.1179	7.45
BUBT	3.402	18	.0057	.29	.0134	.65	.1185	8.15
BUBT	6.805	18	.0253	1.09	.0365	2.06	.1202	8.22
BUBT	13.610	18	.0171	2.07	.0300	3.51	.0911	7.58
BUBT	20.410	12	.0299	2.56	.0511	4.69	.1002	9.69
BUBP	473.15	5	.0248	.564	.0378	1.490	.0980	4.580
DEWP	473.15	5	.0418	.829	.0522	1.310	.2408	16.682
DEWP	423.15	5	.0374	.485	.0466	.340	.2580	7.318
BUBP	423.15	5	.0223	.370	.0307	.110	.1148	2.378

TABLE 4.38. Bubble T Results for Acetone-Water System at Various Pressures(15)

	DATA	AMD(UNIQUAC)		AMD(UNIFAC)		AMD(RAOULT)	
P(ATM)	POINTS	Y	T	Y	T	Y	T
.658	12	.0124	1.06	.0113	.75	.1931	12.73
1.000	13	.0138	.75	.0092	.69	.1641	13.51
3.402	12	.0220	1.18	.0271	1.47	.1837	14.93
6.805	11	.0198	1.42	.0287	2.29	.1659	15.82
13.610	13	.0295	1.93	.0439	3.58	.1547	18.81
17.010	8	.0263	2.24	.0446	3.94	.1571	19.32

TABLE 4.39. VLE Results for Methanol-Water System at Various Pressures(15)

		DATA	AMD(UNIQUAC)		AMD(UNIFAC)		AMD(RAOULT)	
TYPE	P(ATM)	POINTS	X(Y)	T	X(Y)	T	X(Y)	T
BUBT	.967	8	.0347	1.84	.0418	2.47	.0980	6.02
BUBT	1.000	51	.0114	.70	.0130	.33	.6832	4.62
BUBT	3.000	22	.0110	.47	.0058	.94	.0529	4.58
BUBT	5.000	22	.0128	.51	.0087	.80	.0480	4.89
BUBT	8.000	22	.0122	.69	.0085	.53	.0469	4.93
BUBT	11.200	22	.0126	.62	.0094	.42	.0458	4.91
DEWT	11.200	22	.0159	.44	.0122	.71	.0477	5.25

TABLE 4.40 Bubble T Results for Acetone(1)-Water(2) System Using UNIQUAC at 13.610 atm(15)

```
 PRESSURE=  13.610  ATM

                    GIVEN                                                  CALCULATED
               ------------------     ------------------------------------------------
DATA  COMP      X       YE       TE        T            GAMA       FHI        Y
*************************************************************************************
  1    1      .0200   .2890    450.35    455.60        8.7698     .8617      .2312
       2      .9800   .7110                            1.0018     .9338      .7688
  2    1      .0620   .3970    442.05    442.41        6.3942     .8418      .4461
       2      .9380   .6030                            1.0155     .9340      .5539
  3    1      .1080   .4770    437.55    436.06        4.7908     .8328      .5358
       2      .8920   .5230                            1.0432     .9357      .4642
  4    1      .1360   .4950    437.05    433.97        4.1209     .8299      .5641
       2      .8640   .5050                            1.0654     .9366      .4359
  5    1      .1750   .5260    435.65    432.13        3.4301     .8273      .5890
       2      .8250   .4740                            1.1020     .9375      .4110
  6    1      .2440   .5610    433.75    430.32        2.6328     .8249      .6144
       2      .7560   .4390                            1.1818     .9387      .3856
  7    1      .3720   .5930    433.05    428.53        1.8557     .8225      .6435
       2      .6280   .4070                            1.3786     .9405      .3565
  8    1      .3820   .5950    432.25    428.42        1.8158     .8224      .6456
       2      .6180   .4050                            1.3968     .9406      .3544
  9    1      .4890   .6320    431.55    427.38        1.4918     .8211      .6687
       2      .5110   .3680                            1.6248     .9423      .3313
 10    1      .5900   .6690    431.05    426.60        1.2981     .8203      .6940
       2      .4100   .3310                            1.9122     .9445      .3060
 11    1      .6410   .6990    430.95    426.32        1.2258     .8201      .7089
       2      .3590   .3010                            2.0960     .9460      .2911
 12    1      .7520   .7580    430.75    426.11        1.1091     .8207      .7493
       2      .2480   .2420                            2.6387     .9504      .2507
 13    1      .8630   .8500    430.35    427.12        1.0354     .8251      .8118
       2      .1370   .1500                            3.5252     .9588      .1882

              ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=    .0439

              ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=  3.58.
-------------------------------------------------------------------------------------
```

TABLE 4.41.Bubble T Results for acetone(1)-Water(2) System Using UNIFAC at 13.610 atm(15)

```
 PRESSURE=  13.610  ATM

                    GIVEN                                                  CALCULATED
               ------------------     ------------------------------------------------
DATA  COMP      X       YE       TE        T            GAMA       FHI        Y
*************************************************************************************
  1    1      .0200   .2890    450.35    456.31        8.2585     .8628      .2194
       2      .9800   .7110                            1.0017     .9339      .7806
  2    1      .0620   .3970    442.05    443.55        6.0926     .8434      .4312
       2      .9380   .6030                            1.0154     .9339      .5688
  3    1      .1080   .4770    437.55    437.34        4.5805     .8345      .5211
       2      .8920   .5230                            1.0432     .9354      .4789
  4    1      .1360   .4950    437.05    435.34        3.9357     .8317      .5489
       2      .8640   .5050                            1.0658     .9362      .4511
  5    1      .1750   .5260    435.65    433.66        3.2634     .8294      .5723
       2      .8250   .4740                            1.1035     .9370      .4277
  6    1      .2440   .5610    433.75    432.16        2.4810     .8273      .5942
       2      .7560   .4390                            1.1867     .9379      .4058
  7    1      .3720   .5930    433.05    430.83        1.7233     .8255      .6176
       2      .6280   .4070                            1.3938     .9391      .3824
  8    1      .3820   .5950    432.25    430.74        1.6851     .8254      .6194
       2      .6180   .4050                            1.4129     .9392      .3806
  9    1      .4890   .6320    431.55    429.84        1.3822     .8242      .6422
       2      .5110   .3680                            1.6458     .9407      .3578
 10    1      .5900   .6690    431.05    429.10        1.2124     .8233      .6723
       2      .4100   .3310                            1.9191     .9430      .3277
 11    1      .6410   .6990    430.95    428.81        1.1531     .8230      .6917
       2      .3590   .3010                            2.0799     .9448      .3083
 12    1      .7520   .7580    430.75    428.67        1.0654     .8239      .7473
       2      .2480   .2420                            2.4922     .9505      .2527
 13    1      .8630   .8500    430.35    429.80        1.0183     .8297      .8288
       2      .1370   .1500                            3.0036     .9613      .1712

              ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=    .0295

              ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=  1.93
-------------------------------------------------------------------------------------
```

TABLE 4.42. Bubble T Results for Ethanol(1)-Water(2) System Using UNIQUAC at 20.410 atm(15)

```
 PRESSURE=  20.410   ATM

                      GIVEN                                      CALCULATED
               --------------------   ---------------------------------------------
DATA  COMP      X       YE      TE         T           GAMA       FHI        Y
*******************************************************************************
  1     1    .0173   .1080   481.65     481.66       4.1725     .8577     .1083
        2    .9827   .8920                           1.0008     .9135     .8917
  2     1    .0458   .2190   475.95     475.08       3.6404     .8476     .2307
        2    .9542   .7810                           1.0055     .9110     .7693
  3     1    .0527   .2330   475.25     473.82       3.5278     .8457     .2531
        2    .9473   .7670                           1.0072     .9106     .7469
  4     1    .0565   .2400   474.75     473.18       3.4682     .8447     .2646
        2    .9435   .7600                           1.0082     .9104     .7354
  5     1    .0610   .2570   473.85     472.46       3.3997     .8436     .2773
        2    .9390   .7430                           1.0095     .9102     .7227
  6     1    .0917   .3070   471.25     468.43       2.9883     .8373     .3471
        2    .9083   .6930                           1.0207     .9093     .6529
  7     1    .1300   .3650   467.95     465.00       2.5867     .8320     .4058
        2    .8700   .6350                           1.0396     .9088     .5942
  8     1    .1570   .3890   466.75     463.24       2.3605     .8292     .4360
        2    .8430   .6110                           1.0559     .9088     .5640
  9     1    .2180   .4310   464.35     460.44       1.9736     .8249     .4857
        2    .7820   .5690                           1.1009     .9089     .5143
 10     1    .3420   .5090   461.35     457.10       1.5084     .8196     .5534
        2    .6580   .4910                           1.2216     .9100     .4466
 11     1    .4720   .5840   458.85     454.87       1.2559     .8162     .6139
        2    .5280   .4160                           1.3845     .9122     .3861
 12     1    .5360   .6210   458.05     454.02       1.1785     .8150     .6453
        2    .4640   .3790                           1.4772     .9137     .3547

             ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=     .0299

             ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=  2.56
-------------------------------------------------------------------------------
```

TABLE 4.43. Bubble T Results for Ethanol(1)-Water(2) System Using UNIFAC at 20.410 atm(15)

```
 PRESSURE=  20.410   ATM

                      GIVEN                                      CALCULATED
               --------------------   ---------------------------------------------
DATA  COMP      X       YE      TE         T           GAMA       FHI        Y
*******************************************************************************
  1     1    .0173   .1080   481.65     480.07       5.2461     .8554     .1336
        2    .9827   .8920                           1.0011     .9128     .8664
  2     1    .0458   .2190   475.95     472.46       4.3603     .8438     .2670
        2    .9542   .7810                           1.0073     .9101     .7330
  3     1    .0527   .2330   475.25     471.12       4.1826     .8418     .2895
        2    .9473   .7670                           1.0096     .9097     .7105
  4     1    .0565   .2400   474.75     470.45       4.0899     .8407     .3008
        2    .9435   .7600                           1.0109     .9095     .6992
  5     1    .0610   .2570   473.85     469.70       3.9847     .8396     .3132
        2    .9390   .7430                           1.0126     .9093     .6868
  6     1    .0917   .3070   471.25     465.74       3.3789     .8335     .3778
        2    .9083   .6930                           1.0267     .9085     .6222
  7     1    .1300   .3650   467.95     462.60       2.8302     .8286     .4287
        2    .8700   .6350                           1.0498     .9082     .5713
  8     1    .1570   .3890   466.75     461.06       2.5393     .8261     .4541
        2    .8430   .6110                           1.0692     .9082     .5459
  9     1    .2180   .4310   464.35     458.65       2.0703     .8223     .4957
        2    .7820   .5690                           1.1207     .9084     .5043
 10     1    .3420   .5090   461.35     455.65       1.5511     .8176     .5561
        2    .6580   .4910                           1.2522     .9095     .4439
 11     1    .4720   .5840   458.85     453.50       1.2854     .8143     .6147
        2    .5280   .4160                           1.4228     .9116     .3853
 12     1    .5360   .6210   458.05     452.68       1.2047     .8131     .6454
        2    .4640   .3790                           1.5197     .9132     .3546

             ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=     .0511

             ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=  4.69
-------------------------------------------------------------------------------
```

TABLE 4.44. Comparision of Bubble T Results of Acetone(1)-Water(2) System at Various Pressures

DATA POINTS	P(ATM)	AMD(P.R.)IN Y	AMD(ID)IN Y	DAMD
12	.658	.0124	.0124	.0000
13	1.000	.0138	.0142	.0004
12	3.402	.0220	.0229	.0009
11	6.805	.0198	.0234	.0036
13	13.610	.0295	.0335	.0040
8	17.010	.0263	.0310	.0047

P.R.=PENG ROBINSON EQUATION
ID=IDEAL

DAMD=AMD(ID)-AMD(P.R.)

TABLE 4.45 Comparision of Bubble T Results of Ethanol(1)-Water(2) System at Various Pressures

DATA POINTS	P(ATM)	AMD(P.R.)IN Y	AMD(ID)IN Y	DAMD
12	.929	.0029	.0029	.0000
15	1.000	.0036	.0051	.0015
18	3.402	.0061	.0108	.0047
18	6.805	.0407	.0478	.0071
18	13.610	.0231	.0360	.0129
12	20.410	.0313	.0481	.0166

TABLE 4.46. Bubble P Results of Nitrogen(1)-n-Butane(2) Binary System(15)

```
   TEMPERATURE=  310.95 K

                    GIVEN                                         CALCULATED
             --------------------    ------------------------------------------------
DATA COMP     X       YE       PE         P            GAMA       FHI        Y
*********************************************************************************
 1    1     .0250   .7590   15.750     17.544        2.5800     1.0133     .7743
      2     .9750   .2410                             .9997      .7064     .2257
 2    1     .1210   .8900   63.310     73.212        2.5800     1.0129     .9137
      2     .8790   .1100                             .9914      .4369     .0863
 3    1     .1640   .9000  122.400     96.827        2.5800     1.0340     .9173
      2     .8360   .1000                             .9851      .3252     .0627

            ERROR ON Y(1)= ABS(YE(1)-Y(1)/DATA POINTS=    .0188

            ERROR ON P= ABS(PE-P)/DATA POINTS=  12.423
```

TABLE 4.47. Bubble P Results of Hydrogen(1)- n-Hexane(2) Binary System(20)

```
   TEMPERATURE=  277.59 K

                    GIVEN                                          CALCULATED
             --------------------    -------------------------------------------------
DATA COMP     X       YE       PE         P            GAMA       FHI          Y
**********************************************************************************
 1    1     .0280   .9960   34.000     17.474       19.6012     1.0055      .9953
      2     .9720   .0040                             .9996      .8851      .0047
 2    1     .0540   .9980   68.000     33.412       19.6012     1.0120      .9974
      2     .9460   .0020                             .9984      .8047      .0026
 3    1     .0780   .9980  102.000     47.893       19.6012     1.0191      .9981
      2     .9220   .0020                             .9966      .7419      .0019
 4    1     .0990   .9980  136.000     60.356       19.6012     1.0261      .9984
      2     .9010   .0020                             .9944      .6941      .0016

            ERROR ON Y(1)= ABS(YE(1)-Y(1)/DATA POINTS=    .0005

            ERROR ON P= ABS(PE-P)/DATA POINTS=  45.216
```

5 .CONCLUSION AND RECOMMENDATIONS

VLE predictions by UNIQUAC and UNIFAC equations are generally in good agreement with the experimental data. However, from one system to another, one equation sometimes seemed to be better than the other. But, the applicability of UNIFAC to a wide variety of mixtures makes it superior to UNIQUAC for condensable systems. For noncondensable systems UNIFAC can not be applied.

Even though vapor phase nonidealites at low pressures are small and thus they can be neglected, they must be taken into account for pressures higher than atmospheric for accurate VLE predictions. Peng-Robinson is a practical equation to use for vapor phase nonideality predictions.

In conclusion, it can be said that accurate design calculations can be performed either by UNIQUAC or by UNIFAC. If interaction parameters can be predicted accurately for all systems, UNIQUAC and UNIFAC will give good results for all systems. This, of course, requires plentiful accurate experimental data for binary systems.

Recently, UNIFAC has been modified (22,23). In modified UNIFAC, temperature dependence is assumed for interaction parameters and six adjustable parameters are used for one binary group combination. Also, modified UNIFAC has a different combinatorial term. Because of the lack of the binary parameters, it could not be applied in this study. However, VLENC prepared in this study has an option to do calculations by modified UNIFAC, if necessary data are given.

For further study, it is recommended to apply modified UNIFAC and compare the results with UNIQUAC and unmodified UNIFAC. It is, also, recommended to improve the thermodynamic relations to express the behaviour of systems containing noncondensable components.

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APPENDICES

APPENDIX A

ESTIMATION OF THE PHYSICAL PROPERTIES REQUIRED IN THE VLE CALCULATION

A.1. Liquid Molar Volume

Since the liquid molar volume is not usually known as a function of pressure, it is considered as only a function of temperature and composition for engineering purposes. Since the system pressures used in this study were quite lower than the critical pressures, no appreciable error was introduced by assuming that V_i^L in Eq.(2.11) is independent of pressure.

The liquid molar volume was calculated using modified Rackett's equation(24,27):

$$V_i^L = \frac{RT_c}{P_c} Z_a^{\varepsilon} \qquad \text{(A.1.1)}$$

where

$$\varepsilon = 1+(1-T/T_c)^{2/7} \quad \text{for } T/T_c \leq 0.75 \qquad \text{(A.1.2)}$$

$$\varepsilon = 1.60+0.00693026(T/T_c-0.655)^{-1} \text{ for } T/T_c \geq 0.75 \tag{A.1.3}$$

The saturated molar liquid volume and its temperature derivative are continous at T/T_c at 0.75.

Here Z_a is the modified compressibility factor proposed by Rackett. YDATAPP has a list of values of Z_a for a large number of liquids.

A.2. Saturation Vapor Pressure

The vapor pressure of components are predicted by using Antoine vapor pressure :

$$\ln P_i^s = C_1 + \frac{C_2}{T+C_3} \tag{A.2.1}$$

Here P_i^s is in mmHg and T in K. The values of C_1,C_2, and C_3 are listed for a large number of liquids in literature |25|. The file YDATAPP contains most of them.

A.3. Acentric Factor

Acentric factor ω is a measure of the acentricity,i.e., the noncentral nature of intermolecular forces. Acentric factor is defined mathematically by(26).

$$\omega = -\log(P_r^s)_{T_{r=0.7}} - 1.000 \qquad \text{(A.3.1)}$$

For simple fluids $\omega \approx 0$ and for more complex fluids, $\omega > 0$. Here $P_r^s = P_i^s / P_{ci}$.

APPENDIX B

A SAMPLE CALCULATION OF ACTIVITY COEFFICENTS BY UNIFAC

It is desired to obtain the activity coefficients for n-hexanel(1)-benzene(2)system at 350.46 K and X_1= 0.0680. (Table 4.12, 1st point)

n-hexane : CH_3 $\nu^{(1)}_{CH_3} = 2$ CH_2 $\nu^{(1)}_{CH_2} = 4$

benzene : ACH $\nu^{(2)}_{ACH} = 6$

$R_{CH_3} = 0.9011$ $R_{CH_2} = 0.6744$ $R_{ACH} = 0.5313$

$Q_{CH_3} = 0.848$ $Q_{CH_2} = 0.540$ $Q_{ACH} = 0.400$

From Eq.(2.70), we obtain r and q for the componets

$r_1 = 2.0.9011 + 4.0.6744 = 4.4998$

$r_2 = 6.0.5313 = 3.1878$

$q_1 = 2.0.848+4.0.540 = 3.856$

$q_2 = 6.0.4 = 2$

By Eqs.(2.57), (2.58) and (2.61)

$$\Phi_1 = \frac{4.4998x0.0680}{4.4998x0.0680+3.1878x0.932} = 0.0934$$

$\Phi_2 = 0.9066$

$$\ln \Gamma_{CH_3}^{(1)} = \ln \Gamma_{CH_3}^{(1)} \quad (X_{CH_3} = \frac{1}{3}\ ,\ X_{CH_2} = \frac{2}{3})$$

$$\Theta_{CH_3}^{(1)} = \frac{\frac{1}{3} \text{ x } 0.848}{\frac{1}{3} \text{ x } 0.848+\frac{2}{3} \text{x } 0.540} = 0.440$$

$\Theta_{CH_2}^{(2)} = 0.560$

For pure n-hexane, form Eq.(2.74)

$$\ln\Gamma_{CH_3}^{(1)} = 0.848\ |1-\ln(0.440+0.560)-|(\frac{0.440+0.560}{0.440+0.560})|$$

$\ln \Gamma_{CH_3}^{(1)} = 0.0$

$\ln \Gamma_{CH_2}^{(1)} = 0.0$

It is as expected because $\Psi_{CH_3,CH_2} = \Psi_{CH_2,CH_3} = 1.0$

For the mixture at $X_1 = 0.0680$

$$X_{CH_3} = \frac{0.068x2}{0.068x2+0.068x4+0.932x6}$$

$$X_{CH_2} = 0.0227$$

$$X_{CH_2} = 0.0453$$

$$X_{ACH} = 0.932$$

$$\Theta_{CH_3} = \frac{0.0227x0.848}{0.0227.0.848+0.0453x0.540+0.932x0.4}$$

$$\Theta_{CH_3} = 0.0462$$

$$\Theta_1 = \frac{3.856x0.0680}{3.856.0.0680+2.4x0.932} = 0.1049$$

$$\Theta_2 = 0.8951$$

$$l_1 = 5.(4.4998-3.856)-(4.4998-1) = -\ 0.2808$$

$$l_2 = 5.(3.1878-2.4)-(3.1878-1) = 1.7512$$

Subtituting Φ, Θ, l and q into Eq.(2.69) :

$$\ln\gamma_1^C = \ln\frac{0.0934}{0.0680} + 5(3.856)\ln\frac{0.1049}{0.0934} - 0.2808$$

$$\frac{0.0934}{0.0680} - |0.0680.(-0.2808)+0.932.1.7512|$$

$$\ln\gamma_1^C = 0.0598$$

CH_3, CH_2 has the same main group : $CH_2 = \left\}\begin{array}{l} CH_3 \\ CH_2 \\ CH \end{array}\right.$

So, $a_{CH_3,CH_2} = a_{CH_2,CH_3} = 0.0$

$a_{CH_2,ACH} = 61.13$ K $\qquad\qquad a_{ACH,CH_2} = -11.12$

From Eq.(2.76) :

$$\Psi_{CH_2,ACH} = \exp \left|- \frac{61.13}{350.46} \right| = 0.83994$$

$$\Psi_{ACH,CH_2} = \exp \left|- \frac{-11.12}{350.46} \right| = 1.03224$$

$\Theta_{CH_3} = 0.0587 \qquad\qquad \Theta_{ACH} = 0.8951$

From Eq(2.74)

$$\ln\Gamma_{CH_3} = 0.848 | 1 - \ln(0.0462 \dagger 0.0587 \dagger 0.8951.1.03224)$$

$$- | \dagger(\frac{0.462 \dagger 0.0587}{(0.0462 \dagger 0.587 \dagger 0.89591.1.03224)}) |$$

$$\dagger (\frac{0.8951.0.83994}{(0.0462.0.83994 \dagger 0.0587.0.83994 \dagger 0.8951)})$$

$\ln \Gamma_{CH_3} = 0.0890$

$\ln \Gamma_{CH_2} = 0.0567$

From Eq(2.73)

$$\ln\gamma_1^R = 2x(0.0890-0.0)\dagger 4.(0.0567-0.0)$$

$$\ln\gamma_1^R = 0.4048$$

$$\ln\gamma_1 = \ln\gamma_1^C \dagger \ln\gamma_2^R = 0.0598\dagger 0.4048$$

$$\gamma_1 = 1.60$$

by following exactly same procedure for benzene

$$\gamma_2 = 1.00$$

APPENDIX C

PURE COMPONENT AND COMPONENT INTERACTION PARAMETERS

TABLE C.1 UNIQUAC Pure Component Parameters

COMPONENT	R	Q
HYDROGEN	.00	.00
NITROGEN	.00	.00
OXYGEN	.00	.00
CARBON MONOXIDE	.00	.00
ARGON	.00	.00
METHANE	.00	.00
CARBON TETRACHLORIDE	3.33	2.82
CHLOROFORM	2.70	2.34
DIHLOROMETHANE	2.14	1.92
FORMIC ACID	1.54	1.48
NITRO-METHANE	2.01	1.87
METHANOL	1.43	1.43
CARBON DIOXIDE	1.32	1.28
CARBON DISULFIDE	2.08	1.81
TRICHLOROETHYLENE	3.31	2.86
ACETYLENE	1.52	1.39
ACETONITRILE	1.87	1.72
ETHYLENE	1.57	1.49
1,2-DICHLOROETHANE	2.88	2.52
ACETALDEHYDE	1.90	1.80
ACETIC ACID	2.23	2.04
ETHYL IODIDE	2.84	2.38
NITRO-ETHANE	2.68	2.41
ETHANE	1.80	1.70
ETHANOL	2.11	1.97
DIMETHYL AMINE	2.33	2.09
ETYLENE GLYCOL	2.41	2.25
PROPYLENE	2.25	2.02
ACETONE	2.57	2.34
METHYL ACETATE	2.80	2.58
PROPIONIC ACID	2.90	2.58
1-NITROPROPANE	3.36	2.95
2-NITROPROPANE	3.36	2.95
PROPANE	2.48	2.24
N-PROPANOL	2.78	2.51
I-PROPANOL	2.78	2.51
TRIMETHYLAMINE	2.99	2.64
BUTENE-1	2.92	2.56
2-BUTANONE	3.25	2.88
TETRAHYDROFURAN	2.94	2.40
DIOXANE	3.07	2.28
ETHYL ACETATE	3.48	3.12
N-BUTANE	3.15	2.78
I-BUTANE	3.15	2.77
N-BUTANOL	3.45	3.05
I-BUTANOL	3.45	3.05
SEC-BUTANOL	3.45	3.05
TERT-BUTANOL	3.45	3.05
DI-ETHYL ETHER	3.39	3.02
ETHYL CELLOSOLVE	3.70	3.29
DIETHYL AMINE	3.68	3.17
FURFURAL	3.17	2.48
PYRIDINE	3.00	2.16
ISOPRENE	3.36	3.01
CYCLOPENTANE	3.30	2.47
ISOPENTANE	3.82	3.31
N-PENTANE	3.82	3.31
CHLOROBENZENE	3.79	2.84
NITRO-BENZENE	4.13	3.14
BENZENE	3.19	2.40
PHENOL	3.55	2.70
ANILINE	3.72	2.82
CYCLOHEXANONE	4.07	3.11
CYCLOHEXANE	3.97	3.01
HEXENE-1	4.27	3.64
METHYLCYCLOPENTANE	3.97	3.01
CYCLOHEXANOL	4.27	3.51
METHYLISOBUTYLKETONE	4.60	4.03
N-BUTYL ACETATE	4.83	4.20
N-HEXANE	4.50	3.86
2,3-DIMETHYL BUTANE	4.50	3.86
TRIETHYLAMINE	5.01	4.26

... Continued

TABLE C.1 Continued

TOLUENE	3.92	2.97
METHYL CYCLOHEXANE	4.64	3.55
N-HEPTANE	5.17	4.40
STYRENE	4.37	3.30
ETHYL BENZENE	4.60	3.51
M-XYLENE	4.66	3.54
O-XYLENE	4.66	3.54
P-XYLENE	4.66	3.54
N-OCTANE	5.85	4.94
224-TRIMETHYLPENTANE	5.85	4.94
N-DECANE	7.20	6.02
N-HEXADECANE	11.24	9.26
HYDROGEN CHLORIDE	1.00	1.00
WATER	0.92	1.40
HYDROGEN SULFIDE	1.00	1.00
AMMONIA	1.00	1.00
SULFUR DIOXIDE	1.55	1.45
ANISOLE	4.17	3.21
ACRYLONITRILE	2.31	2.05
VINYL ACETATE	3.25	2.90

COMPONENT	Q'
WATER	1.00
METHANOL	0.96
ETHANOL	0.92
N-PROPANOL	0.89
I-PROPANOL	0.89
N-BUTANOL	0.88
I-BUTANOL	0.88
SEC-BUTANOL	0.88
TERT-BUTANOL	0.88
CYCLOHEXANOL	1.78

TABLE C.2 UNIQUAC Interaction Parameters

COMPONET 1	COMPONENT 2	A(1,2)	A(2,1)
ACETONE	ACETIC ACID	461.81	-262.30
ACETONE	ACETONITRILE	-176.38	261.53
ACETONE	BENZENE	-115.95	253.47
ACETONE	CHLOROFORM	-147.83	70.60
ACETONE	CARBON DISULFIDE	103.91	157.31
ACETONE	CARBON TETRACHLORIDE	-92.32	246.68
ACETONE	ETHANOL	404.49	-131.25
ACETONE	FURFURAL	-101.30	195.63
ACETONE	METHANOL	359.10	-96.90
ACETONE	N-HEXANE	-33.08	261.51
ACETONE	N-PENTANE	-22.83	266.31
ACETONE	VINYL ACETATE	-82.48	110.60
ACETONE	WATER	466.36	-56.91
ACETONE	HYDROGEN	218.00	3.23
ACETONE	CARBON MONOXIDE	408.00	.48
ACETONE	METHANE	471.00	-.26
ACRYLONITRIL	ACETONITRILE	573.80	-263.76
ACRYLONITRIL	WATER	575.58	-141.17
ACETIC ACID	ACETALDEHYDE	-212.77	458.43
ACETIC ACID	CHLOROFORM	-98.44	346.43
ACETIC ACID	ETHYL ACETATE	-214.39	426.54
ACETIC ACID	ETHANOL	244.67	-210.53
ACETIC ACID	FORMIC ACID	241.64	-144.58
ACETIC ACID	N-BUTANOL	546.68	-296.30
ACETIC ACID	N-HEPTANE	-8.49	342.57
ACETIC ACID	N-PROPANOL	445.77	299.33
ACETIC ACID	TOLUENE	-67.91	298.09
ACETIC ACID	VINYL ACETATE	-140.18	360.56
ACETIC ACID	WATER	518.98	-296.05
ACETALDEHYDE	VINYL ACETATE	-117.74	243.51
ACETONITRILE	BENZENE	-40.70	229.79
ACETONITRILE	CARBON TETRACHLORIDE	-40.18	458.86
ACETONITRILE	ETHANOL	430.51	68.72
ACETONITRILE	N-HEPTANE	23.71	545.79
ACETONITRILE	WATER	294.10	61.92
ANILINE	METHYLCYCLOPENTANE	54.36	228.71
ANILINE	N-HEXANE	34.82	283.76
ANISOLE	METHANOL	782.28	-48.39
BENZENE	2-BUTANONE	185.55	-144.21
BENZENE	CHLOROFORM	-121.79	83.58
BENZENE	CARBON TETRACHLORIDE	43.39	-37.52
BENZENE	CYCLOPENTANE	33.15	15.19
BENZENE	CYCLOHEXANE	-16.85	66.85
BENZENE	DIOXANE	-197.65	363.78
BENZENE	ETHYL ACETATE	-192.00	248.71
BENZENE	ETHANOL	947.20	-138.90
BENZENE	FURFURAL	-85.00	193.72
BENZENE	I-BUTANOL	861.06	-162.39
BENZENE	I-PROPANOL	854.75	-145.52
BENZENE	METHYLCYCLOPENTANE	-6.47	56.47
BENZENE	METHYL ACETATE	-207.37	278.33
BENZENE	METHANOL	912.41	-50.58
BENZENE	N-BUTANOL	928.90	-181.24
BENZENE	N-HEPTANE	-32.03	87.50
BENZENE	N-HEXANE	-77.13	132.43
BENZENE	N-PROPANOL	928.50	-155.10
BENZENE	1-NITROPROPANE	-246.81	535.16
BENZENE	2-NITROPROPANE	-344.15	794.91
BENZENE	NITRO-ETHANE	46.05	16.61
BENZENE	NITRO-METHANE	163.25	8.34
BENZENE	SEC-BUTANOL	-168.83	784.99
BENZENE	TERT-BUTANOL	-165.40	744.89

... Continued

TABLE C.2 Continued

BENZENE	224-TRIMETHYLPENTANE	-35.12	91.65
BENZENE	TOLUENE	-220.57	330.69
BENZENE	WATER	2057.42	115.13
BENZENE	HYDROGEN	810.00	1.97
BENZENE	CARBON MONOXIDE	1062.00	-1.04
BENZENE	METHANE	473.00	-.38
2-BUTANONE	METHANOL	803.49	-164.22
2-BUTANONE	N-HEPTANE	-75.13	242.53
2-BUTANONE	TOLUENE	-82.85	123.57
2-BUTANONE	WATER	622.84	-55.89
CHLOROFORM	CARBON TETRACHLORIDE	-47.33	76.09
CHLOROFORM	ETHYL ACETATE	24.16	-119.49
CHLOROFORM	ETHANOL	888.68	-203.03
CHLOROFORM	FORMIC ACID	461.38	90.36
CHLOROFORM	METHYL ACETATE	121.17	-187.87
CHLOROFORM	METHANOL	926.31	-143.50
CARBON DISULFIDE	METHANOL	1166.49	138.15
CARBON TETRACHLORIDE	CYCLOHEXANE	124.50	-101.32
CARBON TETRACHLORIDE	ETHANOL	1583.69	-143.68
CARBON TETRACHLORIDE	FURFURAL	476.85	-100.42
CARBON TETRACHLORIDE	METHYLCYCLOPENTANE	161.96	-129.21
CARBON TETRACHLORIDE	METHANOL	1127.95	-29.64
CARBON TETRACHLORIDE	N-BUTANOL	1248.17	-188.77
CARBON TETRACHLORIDE	N-HEPTANE	88.30	-59.13
CARBON TETRACHLORIDE	N-PROPANOL	1075.47	-186.06
CARBON TETRACHLORIDE	1-NITROPROPANE	267.13	-95.68
CARBON TETRACHLORIDE	2-NITROPROPANE	307.25	-134.32
CARBON TETRACHLORIDE	NITRO-ETHANE	295.06	73.06
CARBON TETRACHLORIDE	NITRO-METHANE	398.40	.59
CARBON TETRACHLORIDE	TOLUENE	-168.53	203.67
CYCLOHEXANE	ETHANOL	1269.49	-113.70
CYCLOHEXANE	FURFURAL	265.87	44.32
CYCLOHEXANE	METHYLCYCLOPENTANE	144.37	-118.32
CYCLOHEXANE	METHANOL	1364.12	6.02
CYCLOHEXANE	N-BUTANOL	1360.84	-217.32
CYCLOHEXANE	N-HEXANE	172.73	-145.56
CYCLOHEXANE	N-PROPANOL	1364.65	-168.39
CYCLOHEXANE	NITRO-METHANE	517.19	105.01
CYCLOHEXANE	224-TRIMETHYLPENTANE	-105.65	128.20
CYCLOHEXANE	TOLUENE	83.67	-44.04
1,2-DICHLOROETHANE	ETHANOL	787.17	-104.86
DIETHYL AMINE	METHANOL	676.42	-374.88
DI-ETHYL ETHER	ETHANOL	733.67	-179.02
DIOXANE	WATER	927.26	-328.70
2,3-DIMETHYL BUTANE	METHANOL	1463.90	-7.18
ETHYL ACETATE	ETHYL BENZENE	183.96	-137.27
ETHYL ACETATE	ETHANOL	571.73	-167.61
ETHYL ACETATE	FURFURAL	-19.15	48.52
ETHYL ACETATE	I-PROPANOL	522.07	-190.57
ETHYL ACETATE	METHANOL	579.61	-107.54
ETHYL ACETATE	N-PROPANOL	539.64	-190.31
ETHYL ACETATE	TOLUENE	309.41	-214.26
ETHYL ACETATE	WATER	1081.40	-222.02
ETHANE	N-HEPTANE	264.89	-112.61
ETHANOL	HEXENE-1	-107.26	1222.95
ETHANOL	METHYL CYCLOHEXANE	-117.57	1340.56
ETHANOL	METHYLCYCLOPENTANE	-118.27	1383.93
ETHANOL	METHYL ACETATE	-130.78	573.43
ETHANOL	METHANOL	-292.39	660.19
ETHANOL	N-DECANE	-127.48	1254.65
ETHANOL	N-HEPTANE	-88.48	1180.60
ETHANOL	N-HEXANE	-108.93	1441.57
ETHANOL	N-OCTANE	-123.57	1354.92
ETHANOL	N-PROPANOL	210.95	-67.70

TABLE C.2 Continued

ETHANOL	224-TRIMETHYLPENTANE	-103.21	1443.34
ETHANOL	TOLUENE	-103.87	805.83
ETHANOL	WATER	-71.06	387.38
FURFURAL	224-TRIMETHYLPENTANE	-63.19	385.84
FURFURAL	TOLUENE	244.12	74.87
FORMIC ACID	WATER	924.01	-525.35
I-PROPANOL	N-DECANE	-207.27	1074.76
I-PROPANOL	N-HEPTANE	-173.79	1243.35
I-PROPANOL	N-OCTANE	-166.18	1107.44
I-PROPANOL	224-TRIMETHYLPENTANE	-198.06	994.00
METHYLISOBUTYLKETONE	METHANOL	688.03	-105.94
METHYLISOBUTYLKETONE	PROPIONIC ACID	136.46	-78.49
METHYL CYCLOHEXANE	TOLUENE	210.35	-134.19
METHYLCYCLOPENTANE	N-HEXANE	162.13	-138.34
METHYLCYCLOPENTANE	TOLUENE	89.77	-48.05
METHYL ACETATE	METHANOL	516.12	-95.31
METHANOL	N-HEPTANE	4.84	1325.39
METHANOL	N-HEXANE	-2.66	1636.05
METHANOL	TOLUENE	-27.12	872.31
METHANOL	TRIETHYLAMINE	-186.66	664.29
METHANOL	WATER	-50.82	148.27
METHANOL	HYDROGEN	218.00	3.94
METHANOL	CARBON MONOXIDE	552.00	.83
N-BUTANE	NITROGEN	814.00	-1.67
N-BUTANE	METHANE	731.00	-2.05
N-BUTANOL	N-DECANE	-259.67	1430.77
N-BUTANOL	N-HEPTANE	-251.11	1291.98
N-BUTANOL	N-HEXANE	-159.24	1370.74
N-BUTANOL	N-OCTANE	-236.21	1098.91
N-BUTANOL	WATER	30.64	1098.06
N-DECANE	N-PROPANOL	1137.20	-201.62
N-DECANE	METHANE	150.00	-.24
N-HEPTANE	N-PROPANOL	1083.59	-142.34
N-HEPTANE	TOLUENE	108.24	-72.96
N-HEXANE	N-PROPANOL	1311.01	-152.85
N-HEXANE	2-NITROPROPANE	252.20	-32.95
N-HEXANE	NITRO-ETHANE	230.64	-5.86
N-HEXANE	TOLUENE	220.93	-148.51
N-HEXANE	HYDROGEN	-4.00	2.99
N-HEXANE	NITROGEN	336.00	.07
N-HEXANE	METHANE	94.00	-.06
N-OCTANE	NITRO-ETHANE	333.48	-30.98
N-OCTANE	PROPIONIC ACID	556.12	-183.20
N-OCTANE	CARBON MONOXIDE	1878.00	-3.38
N-PENTANE	METHANE	509.00	-1.32
N-PROPANOL	NITRO-ETHANE	-94.39	574.22
N-PROPANOL	TOLUENE	-195.40	818.34
N-PROPANOL	WATER	23.26	587.18
NITRO-ETHANE	224-TRIMETHYLPENTANE	10.66	236.48
NITRO-ETHANE	WATER	920.08	138.44
PROPANE	METHANE	604.00	-2.01
PROPIONIC ACID	WATER	433.89	-164.67
224-TRIMETHYLPENTANE	TOLUENE	-2.88	19.29
TOLUENE	WATER	1371.36	305.71
VINYL ACETATE	WATER	1541.72	130.05
WATER	HYDROGEN	-880.00	9.97
WATER	NITROGEN	913.00	3.76
HYDROGEN	NITROGEN	.00	.00
HYDROGEN	CARBON MONOXIDE	.00	.00
HYDROGEN	METHANE	.00	.00
NITROGEN	CARBON MONOXIDE	.00	.00
NITROGEN	METHANE	.00	.00
CARBON MONOXIDE	METHANE	.00	.00

TABLE C.3 UNIFAC Functional Group Parameters

MAIN GROUP		SUB GROUP	NO	R	Q
1	CH2	CH3	1	.9011	.848
		CH2	2	.6744	.540
		CH	3	.4469	.228
		C	4	.2195	.000
2	C=C	CH2=CH	5	1.3454	1.176
		CH=CH	6	1.1167	.867
		CH2=C	7	1.1173	.988
		CH=C	8	.8886	.676
		C=C	9	.6605	.485
3	ACH	ACH	10	.5313	.400
		AC	11	.3652	.120
4	ACCH2	ACCH3	12	1.2663	.968
		ACCH2	13	1.0396	.660
		ACCH	14	.8121	.348
5	OH	OH	15	1.0000	1.200
6	CH3OH	CH3OH	16	1.4311	1.432
7	H2O	H2O	17	0.92	1.40
8	ACOH	ACOH	18	.8952	.680
9	CH2CO	CH3CO	19	1.6724	1.488
		CH2CO	20	1.4457	1.180
10	CHO	CHO	21	.9980	.948
11	CCOO	CH3COO	22	1.9031	1.728
		CH2COO	23	1.6764	1.420
12	HCOO	HCOO	24	1.2420	1.188
13	CH2O	CH3O	25	1.1450	1.088
		CH2O	26	0.9183	0.780
		CH-O	27	0.6908	0.468
		FCH2O	28	0.9183	1.100
14	CNH2	CH3NH2	29	1.5959	1.544
		CH2NH2	30	1.3692	1.236
		CHNH2	31	1.1417	0.924
15	CNH	CH3NH	32	1.4337	1.244
		CH2NH	33	1.2070	0.936
		CHNH	34	0.9795	.624
16	(C)3N	CH3N	35	1.1865	0.940
		CH2N	36	0.9597	0.632
17	ACNH2	ACNH2	37	1.0600	0.816
18	PYRIDINE	C5H5N	38	2.9993	2.113
		C5H4N	39	2.8332	1.833
		C5H3N	40	2.6670	1.553
19	CCN	CH3CN	41	1.8701	1.724
		CH2CN	42	1.6434	1.416
20	COOH	COOH	43	1.3013	1.224
		HCOOH	44	1.5280	1.532
21	CCL	CH2CL	45	1.4654	1.264
		CHCL	46	1.2380	0.952
		CCL	47	1.0060	0.724

... Continued

TABLE C.3 Continued

22	CCL2	CH2CL2	48	2.2564	1.988
		CHCL2	49	2.0606	1.684
		CCL2	50	1.8016	1.448
23	CCL3	CHCL3	51	2.8700	2.410
		CCL3	52	2.6401	2.184
24	CCL4	CCL4	53	3.3900	2.910
25	ACCL	ACCL	54	1.1562	0.844
26	CNO2	CH3NO2	55	2.0086	1.868
		CH2NO2	56	1.7818	1.560
		CHNO2	57	1.5544	1.248
27	ACNO2	ACNO2	58	1.4199	1.104
28	CS2	CS2	59	2.0570	1.650
29	CH3SH	CH3SH	60	1.8770	1.676
		CH2SH	61	1.6510	1.368
30	FURFURAL	FURFURAL	62	3.1680	2.481
31	DOH	(CH2OH)2	63	2.4088	2.248
32	I	I	64	1.2640	0.992
33	BR	BR	65	0.9492	0.832
34	C C	CH C	66	1.2920	1.088
		C C	67	1.0613	0.784
35	ME2SO	ME2SO	68	2.8266	2.472
36	ACRY	ACRY	69	2.3144	2.052
37	CLCC	CL(C=C)	70	0.7910	0.724
38	ACF	ACF	71	0.6948	0.524
39	DMF	DMF-1	72	3.0856	2.736
		DMF-2	73	2.6322	2.120
40	CF2	CF3	74	1.4060	1.380
		CF2	75	1.0105	0.920
		CF	76	0.6150	0.460

TABLE C.4 UNIFAC Functional Group Interaction Parameters

GROUP	1	2	3	4	5	6	7	8
1 CH2	.00	-200.00	61.13	76.50	986.50	697.20	1318.00	2789.00
2 C=C	2520.00	.00	340.00	4102.70	639.90	1509.00	634.20	9999.99
3 ACH	-11.12	-94.78	.00	167.00	636.10	637.40	903.80	1397.00
4 ACCH2	-69.70	-269.70	-146.80	.00	803.20	603.30	5695.00	726.30
5 OH	156.40	8694.00	89.60	25.82	.00	-137.10	353.50	286.30
6 CH3OH	16.51	-52.39	-50.00	-44.50	249.10	.00	-181.00	9999.99
7 H2O	300.00	692.70	362.30	377.60	-229.10	289.60	.00	442.00
8 ACOH	310.00	9999.99	2043.00	6245.00	-533.00	9999.99	-540.60	.00
9 CHO	505.70	9999.99	9999.99	9999.99	-404.80	-340.20	232.70	9999.99
10 CCOO	114.80	269.30	85.84	-170.00	245.40	249.60	9999.98	853.60
11 CH2O	83.36	76.44	52.13	65.69	237.70	339.70	-314.70	9999.99
12 CNH2	-30.48	794.00	-44.85	9999.99	-164.00	-481.70	-330.40	9999.99
13 CNH	65.39	-41.32	-22.31	223.00	150.00	-500.40	-448.20	9999.99
14 ACNH2	5339.00	9999.99	650.40	979.80	529.00	5.18	-339.50	9999.99
15 CCN	24.82	34.78	-22.97	-138.40	185.40	157.80	242.80	9999.99
16 COOH	315.30	349.20	62.30	268.20	-151.00	1020.00	-66.17	9999.99
17 CCL	91.46	-24.36	4.68	122.90	562.20	529.00	698.20	9999.99
18 CCL2	34.01	-52.71	121.30	9999.99	747.70	669.90	708.70	9999.99
19 CCL3	36.70	-185.10	288.50	33.61	742.10	649.10	826.80	9999.99
20 CCL4	-78.45	-239.70	-4.70	134.70	856.30	860.10	1201.00	1616.00
21 ACCL	-141.30	-203.20	-237.70	375.70	246.90	661.60	920.40	9999.99
22 CNO2	-32.69	-49.92	10.38	-97.05	341.70	252.60	417.90	9999.99
23 ACNO2	5541.00	9999.99	1825.00	-127.80	561.60	9999.99	360.70	9999.99
24 (C3)N	-83.98	-188.00	-223.90	-109.90	28.60	-406.80	-598.80	9999.99
25 HCOO	90.49	91.65	9999.99	9999.99	191.20	155.70	9999.99	9999.99
26 I	128.00	9999.99	58.68	9999.99	501.30	9999.99	9999.99	9999.99
27 BR	-31.52	9999.99	155.60	291.10	721.90	9999.99	9999.99	9999.99
28 CH3SH	-7.48	9999.99	28.41	9999.99	461.60	382.80	9999.99	9999.99
29 FURFURAL	-25.31	9999.99	157.30	404.30	521.60	9999.99	23.48	9999.99
30 PYRIDINE	-101.60	9999.99	31.87	49.80	-132.20	-378.20	-332.90	-222.20
31 DOH	140.00	9999.99	221.40	150.60	267.60	9999.99	.00	523.00
32 CH2CO	26.76	-89.92	140.10	365.80	164.50	108.70	472.50	9999.99
33 CS2	-52.65	16.62	21.50	40.68	823.50	914.20	1081.00	9999.99
34 C C	-72.88	-184.40	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
35 ME2SO	50.49	9999.99	-2.50	-143.20	-25.87	695.00	-240.00	9999.99
36 ACRY	-165.90	9999.99	9999.99	9999.99	9999.99	9999.99	386.60	9999.99
37 CLCC	41.90	-3.17	-75.67	9999.99	540.90	726.70	9999.99	9999.99
38 ACF	-5.13	9999.99	-237.20	-157.30	649.70	645.90	9999.99	9999.99
39 DMF	-31.95	37.70	-133.90	-240.20	64.16	172.20	-287.10	9999.99
40 CF2	147.30	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99

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TABLE C.4 Continued

GROUP	9	10	11	12	13	14	15	16
1 CH2	677.00	232.10	251.50	391.50	255.70	1245.00	597.00	633.50
2 C=C	9999.99	71.23	289.30	396.00	273.60	9999.99	405.90	730.40
3 ACH	9999.99	5.99	32.14	161.70	122.80	668.20	212.50	537.40
4 ACCH2	9999.99	5688.00	213.10	9999.99	-49.29	764.70	6096.00	603.80
5 OH	441.30	101.10	28.06	83.02	42.70	-348.20	6.71	2199.00
6 CH3OH	306.40	-10.72	-180.60	359.30	266.00	335.50	36.23	-289.50
7 H2O	-257.30	14.42	540.50	48.89	168.00	-213.00	112.60	-14.09
8 ACOH	9999.99	-713.20	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
9 CHO	.00	9999.99	304.10	9999.99	9999.99	9999.99	9999.99	9999.99
10 CCOO	9999.99	.00	-235.70	9999.99	-73.50	9999.99	494.60	660.20
11 CH2O	-7.84	461.30	.00	9999.99	141.70	9999.99	9999.99	664.60
12 CNH2	9999.99	9999.99	9999.99	.00	63.72	9999.99	9999.99	9999.99
13 CNH	9999.99	136.00	-49.30	108.80	.00	9999.99	9999.99	9999.99
14 ACNH2	9999.99	9999.99	9999.99	9999.99	9999.99	.00	-216.80	9999.99
15 CCN	9999.99	-266.60	9999.99	9999.99	9999.99	617.10	.00	9999.99
16 COOH	9999.99	-256.30	338.50	9999.99	9999.99	9999.99	9999.99	.00
17 CCL	-47.51	9999.99	225.40	9999.99	9999.99	9999.99	9999.99	326.40
18 CCL2	9999.99	-132.90	-197.70	9999.99	9999.99	9999.99	9999.99	1821.00
19 CCL3	9999.99	176.50	-20.93	9999.99	9999.99	9999.99	74.04	1346.00
20 CCL4	9999.99	129.50	113.90	261.10	91.13	1302.00	492.00	689.00
21 ACCL	9999.99	-246.30	9999.99	203.50	-104.80	323.30	356.90	9999.99
22 CNO2	9999.99	9999.99	-94.49	9999.99	9999.99	9999.99	9999.99	9999.99
23 ACNO2	9999.99	9999.99	9999.99	9999.99	9999.99	5250.00	9999.99	9999.99
24 (C3)N	9999.99	9999.99	9999.99	38.99	9999.99	9999.99	9999.99	9999.99
25 HCOO	9999.99	-261.10	9999.99	9999.99	9999.99	9999.99	9999.99	-356.30
26 I	9999.99	21.92	474.60	9999.99	9999.99	9999.99	9999.99	9999.99
27 BR	9999.99	9999.99	736.40	9999.99	9999.99	9999.99	9999.99	9999.99
28 CH3SH	9999.99	9999.99	63.71	106.70	9999.99	9999.99	125.70	9999.99
29 FURFURAL	9999.99	-146.30	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
30 PYRIDINE	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	-169.70	-153.70
31 DOH	9999.99	152.00	9.21	9999.99	9999.99	164.40	9999.99	9999.99
32 CH2CO	-37.36	-213.70	5.20	9999.99	9999.99	937.90	481.70	669.40
33 CS2	9999.99	243.8	112.40	9999.99	9999.99	9999.99	335.70	9999.99
34 C C	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	329.10	9999.99
35 ME2SO	9999.99	41.57	-122.10	9999.99	9999.99	9999.99	9999.99	9999.99
36 ACRY	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	-42.31	9999.99
37 CLCC	9999.99	-18.87	-209.30	9999.99	9999.99	9999.99	298.40	298.40
38 ACF	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
39 DMF	9999.99	9999.99	-158.20	9999.99	9999.99	335.60	9999.99	9999.99
40 CF2	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99

TABLE C.4 Continued

	GROUP	17	18	19	20	21	22	23	24
1	CH2	35.93	53.76	24.90	104.30	321.50	661.50	543.00	206.60
2	C=C	96.61	337.10	4583.00	5831.00	959.70	542.10	9999.99	658.80
3	ACH	-18.81	-144.40	-231.90	3.00	538.20	168.10	194.90	90.49
4	ACCH2	-114.10	9999.99	-12.14	-141.30	-126.90	3629.00	4448.00	23.50
5	OH	75.62	-112.10	-98.12	143.10	287.50	61.11	157.10	-323.00
6	CH3OH	-38.32	-102.50	-139.40	-67.80	17.12	75.14	9999.99	53.90
7	H2O	325.40	370.40	353.70	497.50	678.20	220.60	399.50	304.00
8	ACOH	9999.99	9999.99	9999.99	4894.00	9999.99	9999.99	9999.99	9999.99
9	CHO	751.80	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
10	CCOO	9999.99	108.90	-209.70	54.47	629.00	9999.99	9999.99	9999.99
11	CH2O	301.10	137.80	-154.30	47.67	9999.99	95.18	9999.99	9999.99
12	CNH2	9999.99	9999.99	9999.99	-99.81	68.81	9999.99	9999.99	-41.11
13	CNH	9999.99	9999.99	9999.99	71.23	4350.00	9999.99	9999.99	9999.99
14	ACNH2	9999.99	9999.99	9999.99	8455.00	699.10	9999.99	-62.73	9999.99
15	CCN	9999.99	9999.99	-15.62	-54.86	52.31	9999.99	9999.99	9999.99
16	COOH	44.42	-183.40	76.75	211.70	9999.99	9999.99	9999.99	9999.99
17	CCL	.00	108.30	249.20	62.42	464.40	9999.99	9999.99	9999.99
18	CCL2	-84.53	.00	.00	56.33	9999.99	9999.99	9999.99	-141.40
19	CCL3	-157.10	.00	.00	-30.10	9999.99	9999.99	9999.99	-293.70
20	CCL4	11.80	17.97	51.90	.00	475.80	490.90	534.70	-126.00
21	ACCL	-314.90	9999.99	9999.99	-225.40	.00	-154.50	9999.99	1088.00
22	CNO2	9999.99	9999.99	9999.99	-34.68	794.40	.00	533.20	9999.99
23	ACNO2	9999.99	9999.99	9999.99	514.60	9999.99	-85.12	.00	9999.99
24	(C3)N	9999.99	-73.87	-352.90	-8.28	-86.36	9999.99	9999.99	.00
25	HCOO	9999.99	9999.99	-287.20	9999.99	9999.99	9999.99	9999.99	9999.99
26	I	9999.99	-40.82	21.76	48.49	9999.99	64.28	9999.99	9999.99
27	BR	1169.00	9999.99	9999.99	225.80	224.00	125.30	9999.99	9999.99
28	CH3SH	-27.94	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
29	FURFURAL	9999.99	9999.99	48.30	-133.20	9999.99	9999.99	9999.99	9999.99
30	PYRIDINE	9999.99	-351.60	-114.70	-165.10	9999.99	9999.99	9999.99	9999.99
31	DOH	9999.99	9999.99	9999.99	9999.99	9999.99	481.30	9999.99	9999.99
32	CH2CO	-191.70	-284.00	-354.60	-39.20	174.50	137.50	9999.99	9999.99
33	CS2	-73.09	9999.99	-26.06	-60.71	9999.99	9999.99	9999.99	9999.99
34	C C	9999.99	9999.99	9999.99	9999.99	9999.99	174.40	9999.99	9999.99
35	ME2SO	9999.99	-215.00	-343.60	-58.43	9999.99	9999.99	9999.99	9999.99
36	ACRY	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
37	CLCC	201.70	9999.99	85.32	143.20	9999.99	313.80	9999.99	9999.99
38	ACF	9999.99	9999.99	9999.99	-124.60	9999.99	9999.99	9999.99	9999.99
39	DMF	9999.99	9999.99	9999.99	-186.70	9999.99	9999.99	9999.99	9999.99
40	CF2	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99

TABLE C.4 Continued

GROUP	25	26	27	28	29	30	31	32
1 CH2	741.40	335.80	497.50	188.40	354.60	287.60	3025.00	476.40
2 C=C	468.70	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	524.50
3 ACH	9999.99	113.30	-13.59	-10.43	-64.69	-4.50	210.40	25.77
4 ACCH2	9999.99	9999.99	-171.30	9999.99	-20.36	52.80	4975.00	-52.10
5 OH	193.10	313.50	1334.00	147.50	-120.50	170.00	-319.00	34.00
6 CH3OH	193.40	9999.99	9999.99	37.84	9999.99	580.50	9999.99	23.39
7 H2O	9999.99	9999.99	9999.99	9999.99	188.00	459.00	.00	-195.40
8 ACOH	9999.99	9999.99	9999.99	9999.99	9999.99	-637.30	-538.60	9999.99
9 CHO	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	128.00
10 CCOO	372.90	148.30	9999.99	9999.99	202.30	9999.99	-101.70	372.20
11 CH2O	9999.99	-149.50	-202.30	-8.54	9999.99	9999.99	-20.11	52.38
12 CNH2	9999.99	9999.99	9999.99	-70.14	9999.99	9999.99	9999.99	9999.99
13 CNH	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
14 ACNH2	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	125.30	-399.10
15 CCN	9999.99	9999.99	9999.99	21.37	9999.99	134.30	9999.99	-287.50
16 COOH	312.50	9999.99	9999.99	9999.99	9999.99	-313.50	9999.99	-297.80
17 CCL	9999.99	9999.99	-125.90	59.02	9999.99	9999.99	9999.99	286.30
18 CCL2	9999.99	177.60	9999.99	9999.99	9999.99	587.30	9999.99	423.20
19 CCL3	488.90	86.40	9999.99	9999.99	-64.38	-18.98	9999.99	552.10
20 CCL4	9999.99	247.80	41.94	9999.99	546.70	309.20	9999.99	372.00
21 ACCL	9999.99	9999.99	-60.70	9999.99	9999.99	9999.99	9999.99	128.10
22 CNO2	9999.99	304.30	10.17	9999.99	9999.99	9999.99	139.80	-142.60
23 ACNO2	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
24 (C3)N	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
25 HCOO	.00	9999.99	9999.99	4.34	9999.99	9999.99	9999.99	9999.99
26 I	9999.99	.00	9999.99	9999.99	9999.99	9999.99	9999.99	138.00
27 BR	9999.99	9999.99	.00	9999.99	9999.99	9999.99	9999.99	-142.60
28 CH3SH	9999.99	9999.99	9999.99	.00	9999.99	9999.99	9999.99	160.60
29 FURFURAL	9999.99	9999.99	9999.99	9999.99	.00	9999.99	9999.99	317.50
30 PYRIDINE	9999.99	9999.99	9999.99	9999.99	9999.99	.00	9999.99	-51.54
31 DOH	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	.00	9999.99
32 CH2CO	9999.99	53.59	245.20	-46.28	-163.70	165.10	9999.99	.00
33 CS2	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	303.70
34 C C	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	443.60
35 ME2SO	9999.99	9999.99	9999.99	85.70	9999.99	9999.99	535.80	110.40
36 ACRY	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
37 CLCC	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	-8.67
38 ACF	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
39 DMF	9999.99	9999.99	9999.99	-71.00	9999.99	9999.99	-191.70	97.04
40 CF2	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99

TABLE C.4 Continued

GROUP	33	34	35	36	37	38	39	40
1 CH2	153.60	298.90	526.50	689.00	-0.51	125.80	485.30	-2.86
2 C=C	76.30	523.60	9999.99	9999.99	237.30	9999.99	320.40	9999.99
3 ACH	52.07	9999.99	169.90	9999.99	69.11	389.30	245.60	9999.99
4 ACCH2	-9.45	9999.99	4284.00	9999.99	9999.99	101.40	5629.00	9999.99
5 OH	477.00	9999.99	-202.10	9999.99	253.90	44.78	-143.90	9999.99
6 CH3OH	-31.09	9999.99	-399.30	9999.99	-21.22	-48.25	-172.40	9999.99
7 H2O	887.10	9999.99	-139.00	160.80	9999. 99	9999.99	319.00	9999.99
8 ACOH	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
9 CHO	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
10 CCOO	183.00	9999.99	52.08	9999.99	-23.30	9999.99	9999.99	9999.99
11 CH2O	140.90	9999.99	172.10	9999.99	145.60	9999.99	254.80	9999.99
12 CNH2	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
13 CNH	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
14 ACNH2	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	-293.10	9999.99
15 CCN	230.90	-203.00	9999.99	81.57	-19.14	9999.99	9999.99	9999.99
16 COOH	9999.99	9999.99	9999.99	9999.99	-90.87	9999.99	9999.99	9999.99
17 CCL	450.10	9999.99	9999.99	9999.99	-58.77	9999.99	9999.99	9999.99
18 CCL2	9999.99	9999.99	215.00	9999.99	9999.99	9999.99	9999.99	9999.99
19 CCL3	116.60	9999.99	363.70	9999.99	-79.54	9999.99	9999.99	9999.99
20 CCL4	132.20	9999.99	337.70	9999.99	-86.85	215.20	498.60	9999.99
21 ACCL	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
22 CNO2	9999.99	-27.70	9999.99	9999.99	48.40	9999.99	9999.99	9999.99
23 ACNO2	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
24 (C3)N	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
25 HCOO	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
26 I	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
27 BR	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
28 CH3SH	9999.99	9999.99	31.66	9999.99	9999.99	9999.99	76.92	9999.99
29 FURFURAL	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
30 PYRIDINE	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99
31 DOH	9999.99	9999.99	-417.20	9999.99	9999.99	9999.99	302.20	9999.99
32 CH2CO	216.10	-246.60	-44.58	9999.99	-44.42	9999.99	-61.70	9999.99
33 CS2	0.00	9999.99	9999.99	9999.99	-47.37	9999.99	9999.99	9999.99
34 C C	9999.99	0.00	9999.99	9999.99	9999.99	9999.99	-119.80	9999.99
35 ME2SO	9999.99	9999.99	0.00	9999.99	9999.99	9999.99	-97.71	9999.99
36 ACRY	9999.99	9999.99	9999.99	0.00	9999.99	9999.99	9999.99	9999.99
37 CLCC	167.90	9999.99	9999.99	9999.99	0.00	9999.99	9999.99	9999.99
38 ACF	9999.99	9999.99	9999.99	9999.99	9999.99	0.00	9999.99	9999.99
39 DMF	9999.99	6.70	136.60	9999.99	9999.99	9999.99	0.00	9999.99
40 CF2	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	9999.99	0.00

* 9999.99=NOT AVAILABLE

TABLE C.5 Peng-Robinson Interaction Parameters

COMPONENT 1	COMPONENT 2	DEL(1,2)
WATER	METHANE	0.500
WATER	ETHANE	0.500
WATER	PROPANE	0.480
WATER	N-BUTANE	0.480
WATER	N-PENTANE	0.480
WATER	N-HEXANE	0.480
WATER	N-OCTANE	0.480
WATER	1-BUTENE	0.380

APPENDIX D

A SAMPLE OUTPUT OF MAIN PROGRAM VLENC

In this chapter, a sample of interactive use of VLENC is given for acetone-methanol-water ternary system for one data point.

```
 WHAT  TYPE OF CALCULATION DO YOU NEED
 (DEWT/BUBT/DEWP/BUBP)
 BUBT
 ENTER THE NUMBER OF DATA POINTS
 1
 ENTER THE NUMBER OF COMPONENTS
 3
 ARE THE MOLE FRACTIONS STORED IN FILE "DATA" OR
 WILL BE GIVEN INTERACTIVELY

 IF THEY ARE IN "DATA" ENTER " 5 " OTHERWISE " 1 "

 1
 ******** COMPONENT  NAMES ******************

 THE NAMES ARE LISTED ACCORDING TO INCREASE
 IN THE NUMBER OF CARBON ATOMS IN COMPONENTS

 ENTER -TABLE- TO SEE COMPONENTS OTHERWISE ENTER-GO-
 TABLE
--------------------------------------------------------------------------
HYDROGEN                               NITROGEN
OXYGEN                                 CARBON MONOXIDE
ARGON                                  METHANE
CARBON TETRACHLORIDE                   CHLOROFORM
DICHLOROMETHANE                        FORMIC ACID
NITRO-METHANE                          METHANOL
CARBON DIOXIDE                         CARBON DISULFIDE
TRICHLOROETHYLENE                      ACETYLENE
ACETONITRILE                           ETHYLENE
1,2-DICHLOROETHANE                     ACETALDEHYDE
ACETIC ACID                            ETHYL IODIDE
NITRO ETHANE                           ETHANE
ETHANOL                                DIMETHYL AMINE
ETHYLENE GLYCOL                        PROPYLENE
ACETONE                                METHYL ACETATE
PROPIONIC ACID                         1-NITRO PROPANE
PROPANE                                N-PROPANOL
I-PROPANOL                             TRIMETHYLAMINE
BUTENE-1                               2-BUTANONE
TETRAHYDROFURAN                        DIOXANE
--------------------------------------------------------------------------
 ENTER -GO- TO SEE THE OTHERS  OTHERWISE ENTER -OKEY-
 GO



--------------------------------------------------------------------------
ETHYL ACETATE                          N-BUTANE
I-BUTANE                               N-BUTANOL
I-BUTANOL                              SEC-BUTANOL
TERT-BUTANOL                           DI-ETHYL ETHER
DIETHYL AMINE                          FURFURAL
PYRIDINE                               ISOPRENE
CYCLOPENTANE                           ISOPENTANE
N-PENTANE                              CHLOROBENZENE
NITRO-BENZENE                          BENZENE
PHENOL                                 ANILINE
CYCLOHEXANONE                          CYCLOHEXANE
HEXENE-1                               METHYLCYCLOPENTANE
CYCLOHEXANOL                           METHYLISOBUTYLKETONE
N-BUTYL ACETATE                        N-HEXANE
2,3-DIMETHYL BUTANE                    TRIETHYLAMINE
TOLUENE                                METHYL CYCLOHEXANE
N-HEPTANE                              STYRENE
ETHYLBENZENE                           M-XYLENE
```

```
ETHYL BENZENE                                     M-XYLENE
O-XYLENE                                          P-XYLENE
N-OCTANE                                          224-TRIMETHYLPENTANE
------------------------------------------------------------------------------------------
 ENTER -GO- TO SEE THE OTHERS  OTHERWISE ENTER -OKEY-
 GO



------------------------------------------------------------------------------------------
N-DECANE                                          N-HEXADECANE
HYDROGEN CHLORIDE                                 WATER
HYDROGEN SULFIDE                                  AMMONIA
SULFUR DI XIDE                                    ANISOLE
ACRYLONITRILE                                     VINYL ACETATE
------------------------------------------------------------------------------------------
 ENTER THE NAME OF COMPONENT 1
 ACETONE
 ENTER THE NAME OF COMPONENT 2
 METHANOL
 ENTER THE NAME OF COMPONENT 3
 WATER

 CHOOSE ONE OF THE EQUATIONS FOR LIQUID PHASE NONIDEALITY

 1.UNIFAC 2.UNIQUAC 3.RAOULT  4.MODUNIFAC

 ENTER THE NAME OF THE EQUATION
 UNIQUAC
 TC(1)= 5 8.1 PC(1)= 46.4 ZAR(1)= .247
 TC(2)= 5 2.6 PC(2)= 79.9 ZAR(2)= .2318
 TC(3)= 6 7.3 PC(3)= 217.6 ZAR(3)= .238
 NAME(1)= CETONE
 R= 2.57  = 2.34 QP= 2.34
 PU(1 2)= 359.1
 PU(1 3)= 466.36
 NAME(2)= ETHANOL
 PU(2 1)= -96.9
 PU(2 3)= -50.82
 NAME(3)= ATER
 PU(3 1)= -56.91
 PU(3 2)= 148.27
 PROGRAM  TARTS ITERATION FOR BUBBLET CALCULATION
 ***********************************************
 ENTER PRESSURE(IN ATM OR MM HG)
 ENTER UNIT OF THE PRESSURE( ATM OR MM HG)
 1. ATM
 ENTER LIQUID MOLE FRACTION(X) OF ACETONE              AT DATA 1
 .2
 ENTER LIQUID MOLE FRACTION(X) OF METHANOL             AT DATA 1
 .2
 ENTER EXPERIMENTAL VALUE OF VAPOUR MOLE FRACTION
 OF ACETONE            IF AVAILABLE,IF NOT ENTER 0
 .6
 ENTER EXPERIMENTAL VALUE OF VAPOUR MOLE FRACTION
 OF METHANOL           IF AVAILABLE,IF NOT ENTER 0
 .23
 ENTER EXPERIMENTAL VALUE OF TEMPERATURE(IN K OR C OR F)
 IF IT IS NOT AVAILABLE ENTER 0
 (TEMPERATURES FOR ALL DATA POINTS MUST HAVE SAME UNIT)
 ENTER UNIT OF THE TEMPERATURE( K OR F OR C)
 337.95 K
 T= 321.3718604402
 T= 334.8 08617404
 T= 335.5 87361381
 T= 335.5 6244905
```

```
NUMBER OF DATA POINTS=1

DO YOU WANT THE LIST OF THE UNIQUAC  PARAMETERS OF THAT
SYSTEM (YES OR NO)  ?

THEY WIL  BE LISTED IN FILE "ERESULT".
NO



DO YOU WANT CALCULATION WITH A DIFFERENT EQUATION  FROM
UNIQUAC   USING SAME SYSTEM AND DATA YOU HAVE GIVEN(YES OR NO)
YES

 1.UNIFAC 2.UNIQUAC 3.RAOULT 4.MODUNIFAC

 ENTER THE NAME
UNIFAC
TC(1)= 508.1 PC(1)= 46.4 ZAR(1)= .247
TC(2)= 512.6 PC(2)= 79.9 ZAR(2)= .2318
TC(3)= 647.3 PC(3)= 217.6 ZAR(3)= .238
--------------------------------------------------
THE UNIF C METHOD NEEDS FUNCTIONAL GROUPS OF COMPOUNDS
THE CHOICE OF POSSIBLE GROUPS IS ARBITRARY AND LIMITED
WITH THE FOLLOWING GROUPS
CH3    CH2    CH     CH2=CHCH=CH CH=C   CH2=C ACH    AC     ACCH3
ACCH3  AC H2  ACCH   OH     CH3OH H2O    ACOH   CHO    CH3COOCH2COOCH3O
CH3O   CH O   CH-O   FCH2O  CH3NH2CH2NH2CHNH2 CH3NH  CH2NH  CHNH   ACNH2
ACNH2  CH3CN  CH2CN  COOH   HCOOH CH2CL  CHCL   CCL    CH2CL2CHCL2 CCL2
CCL2   CH L3  CCL3   CCL4   ACCL  CH3NO2CH2NO2CHNO2 ACNO2  CH3N   CH2N
CH2N   HCOO   I      BR     CH3SH FURFURPYRID DOH    CO     NH     CL
CL     CH CO  CH2CO  C
--------------------------------------------------
ENTER THE NAME OF UNIFAC GROUPS IN COMPONENT ACETONE
CH3CO
ENTER TH  NUMBER OF GROUPS OF THIS KIND
1
ENTER TH  NAME OF UNIFAC GROUPS IN COMPONENT ACETONE
CH3
ENTER THE NUMBER OF GROUPS OF THIS KIND
1
ENTER TH  NAME OF UNIFAC GROUPS IN COMPONENT ACETONE
END
--------------------------------------------------
THE UNIF C METHOD NEEDS FUNCTIONAL GROUPS OF COMPOUNDS
THE CHOICE OF POSSIBLE GROUPS IS ARBITRARY AND LIMITED
WITH THE FOLLOWING GROUPS
CH3    CH2    CH     CH2=CHCH=CH CH=C   CH2=C ACH    AC     ACCH3
ACCH3  AC H2  ACCH   OH     CH3OH H2O    ACOH   CHO    CH3COOCH2COOCH3O
CH3O   CH2O   CH-O   FCH2O  CH3NH2CH2NH2CHNH2 CH3NH  CH2NH  CHNH   ACNH2
ACNH2  CH3CN  CH2CN  COOH   HCOOH CH2CL  CHCL   CCL    CH2CL2CHCL2 CCL2
CCL2   CH L3  CCL3   CCL4   ACCL  CH3NO2CH2NO2CHNO2 ACNO2  CH3N   CH2N
CH2N   HCOO   I      BR     CH3SH FURFURPYRID DOH    CO     NH     CL
CL     CH CO  CH2CO  C
--------------------------------------------------
ENTER THE NAME OF UNIFAC GROUPS IN COMPONENT METHANOL
CH3OH
ENTER THE NUMBER OF GROUPS OF THIS KIND
1
ENTER THE NAME OF UNIFAC GROUPS IN COMPONENT METHANOL
END
--------------------------------------------------
THE UNIFAC METHOD NEEDS FUNCTIONAL GROUPS OF COMPOUNDS
THE CHOICE OF POSSIBLE GROUPS IS ARBITRARY AND LIMITED
WITH THE FOLLOWING GROUPS
CH3    CH2    CH     CH2=CHCH=CH CH=C   CH2=C ACH    AC     ACCH3
ACCH3  ACCH2  ACCH   OH     CH3OH H2O    ACOH   CHO    CH3COOCH2COOCH3O
```

```
ACCH3  AC.H2  ACCH   OH     CH3OH  H2O    ACOH   CHO    CH3COOCH2COOCH3O
CH3O   CH2O   CH-O   FCH2O  CH3NH2CH2NH2CHNH2  CH3NH  CH2NH  CHNH   ACNH2
ACNH2  CH3CN  CH2CN  COOH   HCOOH  CH2CL  CHCL   CCL    CH2CL2CHCL2  CCL2
CCL2   CHCL3  CCL3   CCL4   ACCL   CH3NO2CH2NO2CHNO2  ACNO2  CH3N   CH2N
CH2N   HCOO   I      BR     CH3SH  FURFURPYRID  DOH    CO     NH     CL
CL     CH CO  CH2CO  C
--------------------------------------------------------
ENTER TH  NAME OF UNIFAC GROUPS IN COMPONENT WATER
H2O
ENTER THE NUMBER OF GROUPS OF THIS KIND
1
ENTER TH  NAME OF UNIFAC GROUPS IN COMPONENT WATER
END
TABLE(1  1 1  1)= 0.
TABLE(1  1 1  2)= 26.76
TABLE(1    2  1)= 108.7
TABLE(1  1 3  1)= 472.5
TABLE(1  2 1  1)= 476.4
TABLE(1  2 1  2)= 0.
TABLE(1  2 2  1)= 697.2
TABLE(1  2 3  1)= 1318.
TABLE(2  1 1  1)= 23.39
TABLE(2  1 1  2)= 16.51
TABLE(2  1 2  1)= 0.
TABLE(2  1 3  1)= -181.
TABLE(3  1 1  1)= -195.4
TABLE(3  1 1  2)= 300.
TABLE(3  1 2  1)= 289.6
TABLE(3    3  1)= 0.
PROGRAM STARTS ITERATION FOR BUBBLET CALCULATION
*****************************************
T= 325.9 38802877
T= 333.2714743085
T= 338.8 81975718
T= 338.8574503938
NUMBER OF DATA POINTS=1

DO YOU WANT THE LIST OF THE UNIFAC   PARAMETERS OF THAT
SYSTEM (YES OR NO)  ?

THEY WILL BE LISTED IN FILE "ERESULT".
NO



DO YOU WANT CALCULATION WITH A DIFFERENT EQUATION  FROM
UNIFAC    USING SAME SYSTEM AND DATA YOU HAVE GIVEN(YES OR NO)
YES

 1.UNIFAC 2.UNIQUAC 3.RAOULT 4.MODUNIFAC

 ENTER THE NAME
RAOULT
TC(1)= 5 8.1 PC(1)= 46.4 ZAR(1)= .247
TC(2)= 512.6 PC(2)= 79.9 ZAR(2)= .2318
TC(3)= 647.3 PC(3)= 217.6 ZAR(3)= .238
PROGRAM STARTS ITERATION FOR BUBBLET CALCULATION
*****************************************
T= 343.4 34870944
T= 350.2 12763293
T= 350.4423706407
T= 350.4 29109649
NUMBER OF DATA POINTS=1


DO YOU WANT CALCULATION WITH A DIFFERENT EQUATION  FROM
```

```
DO YOU WANT CALCULATION WITH A DIFFERENT EQUATION FROM
RAOULT    USING SAME SYSTEM AND DATA YOU HAVE GIVEN(YES OR NO)
NO

DO YOU NEED ANOTHER CALCULATION (YES,NO)
NO
--------------------------------------------------
THE RESULTS OF THE CALCULATION(S) ARE STORED
IN THE FILE "ERESULT"

THE RESULTS OF THE ITERATIONS IN THE CALCULATIONS
ARE STORED IN THE FILE  "PUTPUT"
--------------------------------------------------


        TABLE(    )       VLE CALCULATION RESULTS

    1.ACETONE                2.METHANOL              3.WATER

        TYPE: BUBT,

        LIQUID PHASE NONIDEALITY IS  CALCULATED BY UNIQUAC  EQUATION
        VAPOUR PHASE NONIDEALITY IS CALCULATED BY PENG ROBINSON EQUATION

 PRESSURE=   1.000  ATM

                  GIVEN                                   CALCULATED
           --------------------   ------------------------------------------
DATA COMP    X     YE      TE       T         GAMA      FHI       Y        E%
*******************************************************************************
 1   1    .2000  .6000   337.95   336.51     2.3595    .9743    .5911    -1.43
     2    .2000  .2300                       1.2134    .9827    .2318      .79
     3    .6000  .1700                       1.2780    .9911    .1770     4.13

        ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=   .0089

        ERROR ON Y(2)= ABS(Y(2)-YE(2))/DATA POINTS=   .0018

        ERROR ON Y(3)= ABS(Y(3)-YE(3))/DATA POINTS=   .0070

        ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=  1.4438

        TABLE(    )       VLE CALCULATION RESULTS

    1.ACETONE                2.METHANOL              3.WATER

        TYPE: BUBT

        LIQUID PHASE NONIDEALITY IS  CALCULATED BY UNIFAC   EQUATION
        VAPOUR PHASE NONIDEALITY IS CALCULATED BY PENG ROBINSON EQUATION

 PRESSURE=   1.000  ATM

                  GIVEN                                   CALCULATED
           --------------------   ------------------------------------------
DATA COMP    X     YE      TE       T         GAMA      FHI       Y        E%
*******************************************************************************
 1   1    .2000  .6000   337.95   339.86     2.0370    .9743    .5662    -5.63
     2    .2000  .2300                       1.0491    .9830    .2281     -.84
     3    .6000  .1700                       1.2789    .9911    .2057    21.02

        ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=   .0338

        ERROR ON Y(2)= ABS(Y(2)-YE(2))/DATA POINTS=   .0019

        ERROR ON Y(3)= ABS(Y(3)-YE(3))/DATA POINTS=   .0357
```

```
        ERROR ON Y(3)= ABS(Y(3)-YE(3))/DATA POINTS=   [illegible]

        ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS=  1.9075


       TABLE(     )          VLE CALCULATION RESULTS

    1.AC:TONE                  2.METHANOL                 3.WATER

        TYPE: BUBT

        CALCULATIONS ARE PERFORMED BY RAOULT"S LAW

  PRESSURE=    1.000  ATM

                    GIVEN                                     CALCULATED
           --------------------   ------------------------------------------
)ATA COMP    X      YE      TE       T           GAMA      FHI      Y        E%
*******************************************************************************
  1    1   .2000  .6000  337.95  351.44       1.0000   1.0000   .4021  -32.98
       2   .2000  .2300                        1.0000   1.0000   .3362   46.19
       3   .6000  .1700                        1.0000   1.0000   .2617   53.93

        ERROR ON Y(1)= ABS(Y(1)-YE(1))/DATA POINTS=   .1979

        ERROR ON Y(2)= ABS(Y(2)-YE(2))/DATA POINTS=   .1062

        ERROR ON Y(3)= ABS(Y(3)-YE(3))/DATA POINTS=   .0917

        ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS= 13.4929

--------------------------------------------------------------------------------

--------------------------------------------------------------------------------
17.45.09.UCLP, BU, P03     ,         0.399KLNS.
```

APPENDIX E

DESCRIPTION AND LISTING OF VLENC AND ITS SUBROUTINES

1. Main Program VLENC

Interactively designed program VLENC organizes the relationship among subroutines. It interactively reads the system's components, the type of calculations and options for liquid phase nonideality calculations. Next, calling subroutine INPUT, it transfers the pure component and binary interaction parameters to the subroutines of interest. For liquid phase nonideality, it has mainly three options, UNIFAC,UNIQUAC and modified UNIFAC. It is also able to make predictions with Raoult's law. VLENC has the ability to reperform the calculations with different equations representing the liquid phase nonideality, without reentering the input data.

2. Subroutines DEWT,BUB T,DEWP and BUBP

These four subroutines perform dew point temperature, bubble point temperature, dew point pressure and bubble point pressure calculations using the calculational methods described in Chapter 3. They interactively read required mole fractions, pressure of temperature and, if available, the experimental values of unknown variables. The pure component and interaction parameters of the system in interest are transferred through the main program. Then, these subroutines calculate unknown mole fractions and temperature or pressure by calling subroutines VAPS,CONST,FUGAC,RFUGAC,UNIQUAC or UNIFAC. At the end of the calculations, they find percentage errors and absolute mean deviations between predicted and experimental values of unknown variables.

3. Subroutien VAPS

It calculates saturated vapor pressures by using Antoine Equation as it is given in Appendix A.1.

4. Subroutine CONST

CONST calculates the parameters of Peng-Robinson Equation required for both in FUGAC and RFUGAC subroutines. If experimental data are not available for acentric factor, it calls function ACEF in order to obtain a predicted value.

5. Subroutine FUGAC

It finds the fugacity coefficient of thecomponent in interest by substituting compressibility factor Z, obtained from subroutine ROOT into Eq.(2.35).

6. Subroutine RFUGAC

It calculates saturated fugacity coefficient for pure component using Eq.(2.34) by calling subroutine ROOT to calculate compressibility factor Z, of that component.

7. Subroutine UNIQUAC

It uses Eq.(2.60) for condensable component activity coefficient. For a noncondensable component, it calls subroutine RFUGNC and uses Eq.(2.63).

8. Subroutine UNIFAC

It finds UNIFAC activity coefficients using Eqs.(2.68)-(2.76). It is not able to calculate activity coefficients of noncondensable components. This subroutine is also able to find the activity coefficients of modified UNIFAC equation, whenever interaction parameters are available.

9. Subroutine LMV

It finds liquid molar volumes using modified Rackett Equation as given in Appendix A.2.

10. Subroutine INPUT

It reads and loads physcial properties of the components in file YDATAPP, UNIQUAC parameters in file YDATAUQ, and UNIFAC parameters in file YDATUM. It chooses the parameters of the system of interest by comparing the names of the components with the names given in data files.

11. Subroutine OUT

It prints the names of components, the system conditions and UNIQUAC or UNIFAC parameters of the system in interest.

12. Subroutine ROOT

It finds compressibility factor Z in Eq(2.23) both for the mixture and for pure components using Newton-Raphson iteration method.

13. Subroutine RFUGNC

It finds the hypothetical standar state fugacity for noncondensable components from Eq.(2.65)

14. Subroutine ACEF

Subroutine ACEF, finds the acentric factor of a component, which is not available in the data YDATAPP, by using the equation given in Appendix A.3.

15. Subroutine FINDR

It finds the code number of the UNIFAC group in interest in data file YDATUM.

The Main Variables Used in the Programs

ANTA,ANTB,ANTC	Constants of Antoine equation
DEL	Peng-Robinson interaction parameter
FHI	Fugacity coefficient of a component in solution.
FHS	Saturation fugacity coefficient of a pure component
GAMA	Activity coefficient.
HC	Henry's constant.
N	Number of data points
NN	Number of components
OMEGA	Acentric factor
P	Pressure
PC	Critical pressure
PS	Saturation vapor pressure
PU	UNIQUAC energy interaction parameter
QX	UNIQUAC surface parameter in combinatorial part
QPX	UNIQUAC surface parameter in residual part.
QB	UNIFAC group surface parameter
RX	UNIQUAC volume parameter
RB	UNIFAC group volume parameter

T	Temperature
TABLE	UNIFAC group interaction parameter
TC	Critical temperature
VL	Liquid molar volume
X	Liquid mole fraction
XE	Experimental liquid mole fraction
Y	Vapor mole fraction
YE	Exeperimental mole fraction
Z	Compressibility factor
ZAR	Rackett equation parameter

```
      PROGRAM VLE(OUTPUT,DATA,YDATAPP,YDATAUQ,YDATUM,ERESULT,YLIST,PUTPUT,INPUT,
     +TAPE2=YDATAPP,TAPE3=YDATAUQ,TAPE4=YDATUM,TAPE6=ERESULT,TAPE8=YLIST,TAPE1=
     +PUTPUT,TAPE5=DATA,TAPE7=INPUT)
C
C     VAPOUR-LIQUID EQUILIBRIUM  CALCULATIONS
C
      PARAMETER (K=9)
      PARAMETER (MMR=4)
      DIMENSION RQ(63,2),DEL(K,K),ZAR(K),COMP(63)
      DIMENSION ANTA(K),ANTB(K),ANTC(K)
      COMMON/CONV/ TC(K),PC(K),OMEGA(K)
      COMMON/UNIQ/ R(K),Q(K),QP(K),PU(K,K)
      COMMON/UNIFAC1/RB(K,MMR),QB(K,MMR),TABLE(63,63),KONT(K)
      COMMON/UNIFAC2/ITAB(K,MMR),KQR(K,MMR),MNR(K)
      COMMON NAME(K),LFED,TYPE
      CHARACTER*6 COMP
      CHARACTER*35 COMN1,COMN2
      CHARACTER*20 NAME
      CHARACTER*9  LFED,TYPE,RDEC,DEC,HR,PTD
C
C     INTERACTIVE DATA INPUT SECTION
C
 55   RD=0
      INFR=0
      NRA=0
      PRINT*,'WHAT  TYPE OF CALCULATION DO YOU NEED'
      PRINT*,'(DEWT,BUBT,DEWP,BUBP)'
      READ(*,1) TYPE
      PRINT*,TYPE
 1    FORMAT(A)
      PRINT*,'ENTER THE NUMBER OF DATA POINTS'
      READ*,N
      PRINT*,N
      PRINT*,'ENTER THE NUMBER OF COMPONENTS'
      READ*,NN
      PRINT*,NN
      PRINT*,'ARE THE MOLE FRACTIONS STORED IN FILE "DATA" OR  '
      PRINT*,'WILL BE GIVEN INTERACTIVELY'
      PRINT*,' '
      PRINT*,'IF THEY ARE IN "DATA" ENTER " 5 " OTHERWISE " 7 "'
      READ*,IOD
      PRINT*,' '
      PRINT*,IOD
      CALL PF('GET','YLIST')
      PRINT*,'******** COMPONENT  NAMES *******************'
      PRINT*,' '
      PRINT*,'THE NAMES ARE LISTED ACCORDING TO INCREASE   '
      PRINT*,'IN THE NUMBER OF CARBON ATOMS IN COMPONENTS  '
      PRINT*,' '
      PRINT*,'ENTER -TABLE- TO SEE COMPONENTS OTHERWISE ENTER-GO-'
      READ(*,1)HR
      PRINT*,HR
      IF(HR.EQ.'GO')GO TO 485
      WRITE(*,445)
      READ(8,*) TC1
      DO 195 I=1,TC1
      READ(8,12) COMN1,COMN2
      WRITE(*,12) COMN1,COMN2
      AAA=I/20.0
      JIK=I/20
      IF(JIK.NE.AAA)GO TO 195
```

```
      WRITE(*,445)
      PRINT*,'ENTER -GO- TO SEE THE OTHERS  OTHERWISE ENTER -OKEY-'
      READ(*,1) HR
      PRINT*,HR
      IF(HR.EQ.'OKEY')GO TO 485
      DO 25 J=1,3
 25   PRINT*,'                                                    '
      WRITE(*,445)
195   CONTINUE
 12   FORMAT(2(A35))
      WRITE(*,445)
445   FORMAT(76('-'))
485   DO 200 I=1,NN
      PRINT*,'ENTER THE NAME OF COMPONENT ',I
      READ(*,1) NAME(I)
      PRINT*,NAME(I)
200   CONTINUE
      PRINT*,' '
      PRINT*,'CHOOSE ONE OF THE EQUATIONS FOR LIQUID PHASE NONIDEALITY'
      PRINT*,'                   '
      PRINT*,'1.UNIFAC 2.UNIQUAC 3.RAOJLT  4.MODUNIFAC     '
      PRINT*,'                                             '
      PRINT*,'ENTER THE NAME OF THE EQUATION               '
      READ(*,1) LFED
      PRINT*,LFED
175   IF(LFED.EQ.'UNIFAC'.OR.LFED.EQ.'MODUNIFAC')GO TO 24
      IF(LFED.EQ.'RAOULT') GO TO 28
      LFD=1
      GO TO 152
 24   LFD=2
      MU=0
      IF(LFED.EQ.'MODUNIFAC')MU=1
      GO TO 152
 28   LFD=3
C
C     READ THE REQUIRED DATA BY CALLING SUBROUTINE INPUT
C
152   CALL INPUT(ANTA,ANTB,ANTC,ZAR,DEL,LFD,NN,SCN,NRA,COMP)
C
C     CHOOSE ONE OF THE OPTIONS
C
      IF(LFD.EQ.2.AND.LFED.NE.'MODUNIFAC')LFED='UNIFAC'
      IF(TYPE.EQ.'DEWT')GO TO 3
      IF(TYPE.EQ.'BUBT')GO TO 4
      IF(TYPE.EQ.'BUBP')GO TO 5
      IF(TYPE.EQ.'DEWP')GO TO 7
      PRINT*,'THE NAME FOR CALCULATION IS WRONG,ENTER AGAIN'
      GO TO 55
  7   CALL DEWP(N,NN,ANTA,ANTB,ANTC,DEL,LFD,ZAR,RD,MU,IOD,COMP)
      GO TO 50
  3   CALL DEWT(N,NN,ANTA,ANTB,ANTC,DEL,LFD,ZAR,RD,MU,IOD,COMP)
      GO TO 50
  4   CALL BUBT(N,NN,ANTA,ANTB,ANTC,DEL,LFD,ZAR,RD,MU,IOD,COMP)
      GO TO 50
  5   CALL BUBP(N,NN,ANTA,ANTB,ANTC,DEL,LFD,ZAR,RD,MU,IOD,COMP)
 50   IF(LFED.EQ.'RAOULT') GO TO 350
      PRINT*,' '
      PRINT*,'DO YOU WANT THE LIST OF THE ',LFED,'PARAMETERS OF THAT'
      PRINT*,'SYSTEM (YES OR NO)  ? '
      PRINT*,' '
      PRINT*,'THEY WILL BE LISTED IN FILE "ERESULT".'
      READ(*,1)PTD
      PRINT*,PTD
      IF(PTD.EQ.'YES')CALL OUT(NN,1,COMP)
350   IF(LFED.EQ.'RAOULT')WRITE(6,5555)
5555  FORMAT(/,80('-'),/,80('_'))
```

```
      IF(INFR.GE.3)GO TO 49
 112  PRINT*,' '
      PRINT*,' '
      PRINT*,' '
      PRINT*,'DO YOU WANT CALCULATION WITH A DIFFERENT EQUATION  FROM '
      PRINT*,LFED,' USING SAME SYSTEM AND DATA YOU HAVE GIVEN(YES OR NO)'
      READ(*,1) RDEC
      PRINT*,RDEC
      IF(RDEC.EQ.'NO')GO TO 49
      IF(LFED.EQ.'UNIFAC'.OR.LFED.EQ.'MODUNIFAC')NRA=1
      PRINT*,'                                                         '
      PRINT*,' 1.UNIFAC 2.UNIQUAC 3.RAOULT 4.MODUNIFAC                 '
      PRINT*,' '
      PRINT*,' ENTER THE NAME'
      READ(*,1) LFED
      PRINT*,LFED
      RD=1
      INFR=INFR+1
      GO TO 175
 49   PRINT*,' '
      PRINT*,'DO YOU NEED ANOTHER CALCULATION (YES,NO)'
      READ(*,1) DEC
      PRINT*,DEC
      IF(DEC.EQ.'NO') GO TO 555
      GO TO 55
 555  PRINT*,'_____________________________________________________'
      PRINT*,'THE RESULTS OF THE CALCULATION(S) ARE STORED'
      PRINT*,'IN THE FILE "ERESULT" '
      PRINT*,' '
      PRINT*,'THE RESULTS OF THE ITERATIONS IN THE CALCULATIONS'
      PRINT*,'ARE STORED IN THE FILE  "PUTPUT"'
      PRINT*,'---------------------------------------------------- '
      STOP
      END
C     ----------------------------------------------------------------
C
      SUBROUTINE  DEWT(N,NN,ANTA,ANTB,ANTC,DEL,LFD,ZAR,RD,MU,IOD,COMP)
C
C     -----------------------------------------------------------------
      PARAMETER(K=9)
      PARAMETER(MMR=4)
      DIMENSION XU(K),XQ(K),GAMA(K),RQ(63,2),ZAR(K),VL(K),COMP(63)
      DIMENSION Y(K),XE(K),ANTA(K),ANTB(K),ANTC(K),HC(K),TE(100)
      DIMENSION YA(K,100),XEA(K,100),XQO(K),YE(K),YEA(K,100),X(K)
      DIMENSION A(K),B(K),Z(K),APR(K),BPR(K),XA(K,100),SED(K)
      DIMENSION FIL(K),EY(K),EX(K),VK(K),CX(K),DEL(K,K),PS(K)
      COMMON/CONV/ TC(K),PC(K),OMEGA(K)
      COMMON/UNIQ/ R(K),Q(K),QP(K),PU(K,K)
      COMMON/UNIFAC1/RB(K,MMR),QB(K,MMR),TABLE(63,63),KONT(K)
      COMMON/UNIFAC2/ITAB(K,MMR),KQR(K,MMR),MNR(K)
      COMMON/FUGV/APRM,BPRM,APRIJ(K,K),FHI(K)
      COMMON/RFUGV/FHS(K)
      COMMON NAME(K),LFED,TYPE
      CHARACTER*6 CM1,PUI,TUI,COMP
      CHARACTER*20 NAME
      CHARACTER*9  LFED,TYPE
C
C     VAPOUR AND LIQUID DATA
C
      PRINT*,'PROGRAM STARTS ITERATION FOR DEWT CALCULATION'
      PRINT*,'*********************************************'
      EPS=0.00001
      DO 56 I=1,NN
 56   WRITE(1,1)NAME(I)
      WRITE(1,1)LFED
      WRITE(1,*)
```

```
      N1=N
      IF(RD.EQ.1)GO TO 177
      PRINT*,'ENTER PRESSURE (IN ATM OR MM HG)'
      READ(*,*) P
      PRINT*,'ENTER UNIT OF THE PRESSURE ("ATM" OR "MM HG")'
      READ(*,1) PUI
    1 FORMAT(A)
      IF(PUI.EQ.'MM HG')P=P/760
      PRINT*,P,' ATM'
  177 CALL OUT(NN,0,COMP)
      WRITE(6,1001) P
      DO 302 I=1,NN
  302 SED(I)=0.0
      SET=0.0
      DO 212 M=1,N
      SUMXX=0.0
      SUMYY=0.0
      IF(RD.EQ.1)GO TO 155
      DO 112 I=1,NN-1
      PRINT*,'ENTER VAPOUR MOLE FRACTION(Y) OF ',NAME(I),'AT DATA',M
      READ(IOD,*) YA(I,M)
  112 PRINT*,YA(I,M)
      DO 114 I=1,NN-1
      PRINT*,'ENTER EXPERIMENTAL VALUE OF LIQUID MOLE FRACTION'
      PRINT*, 'OF ',NAME(I),'IF AVAILABLE,IF NOT ENTER 0'
      READ(IOD,*) XEA(I,M)
      PRINT*,XEA(I,M)
      IF(XEA(I,M).EQ.0) GO TO 155
  114 CONTINUE
      PRINT*,'ENTER EXPERIMENTAL VALUE OF TEMPERATURE (IN K OR F OR C)'
      PRINT*,'IF IT IS NOT AVAILABLE ENTER 0'
      PRINT*,'(TEMPERATURES FOR ALL DATA POINTS MUST HAVE SAME UNIT)'
      READ(IOD,*) TE(M)
      IF(M.GT.1) GO TO 123
      PRINT*,'ENTER UNIT OF THE TEMPERATURE(K OR F OR C)'
      READ(IOD,1)TUI
  123 IF(TUI.EQ.'F')TE(M)=(TE(M)+459.67)/1.8
      IF(TUI.EQ.'C')TE(M)=TE(M)+273.15
      PRINT*,TE(M),' K'
  155 DO 139 I=1,NN-1
      Y(I)=YA(I,M)
      XE(I)=XEA(I,M)
      SUMYY=SUMYY+Y(I)
      SUMXX=SUMXX+XE(I)
  139 CONTINUE
      Y(NN)=1.0-SUMYY
      XE(NN)=1.0-SUMXX
      IF(XEA(1,M).EQ.0.0)XE(NN)=0.0
C
C     ITERATION FOR DEWT CALCULATION
C
      DO 2 I=1,NN
      X(I)=Y(I)
    2 CONTINUE
      T=400
      CR=82.057
      TLL=100.
      IRP=0
      NNN=2
      IN=0
  100 IN=IN+1
      RT=82.057*T
  101 DO 149 J=1,NNN
      IF(J.EQ.2)T=T+1
      CALL VAPS(ANTA,ANTB,ANTC,T,PS,NN)
      IF(LFD.EQ.3) GO TO 471
```

```
      CALL CONST(A,B,APR,BPR,NN,T,P,CR,PS,ANTA,ANTB,ANTC)
      CALL LMV(PC,TC,ZAR,VL,T,NN)
      CALL RFUGAC(Z,A,B,NN,T)
      CALL FUGAC(ZMIX,Y,APR,BPR,NN,T,P,CR,DEL)
      GO TO (72,73),LFD
   72 CALL UNIQUAC(X,T,NN,GAMA,HC)
      GO TO 75
   73 CALL UNIFAC(X,NN,T,GAMA,MU)
   75 SUMX=0.
      DO 5 I=1,NN
      PCL=EXP(VL(I)*(P-PS(I))/RT)
      FIY=FHI(I)*P
      FILMP=GAMA(I)*PS(I)*FHS(I)*PCL
      IF(T/TC(I).GT.1.3)FILMP=HC(I)
      IF(T/TC(I).GT.1.3)TLL=0.0
      VK(I)=FILMP/FIY
      CX(I)=Y(I)/VK(I)
      SUMX=SUMX+CX(I)
    5 CONTINUE
      IF(SUMX.GT.10000.OR.SUMX.LT.0.00001)GO TO 414
      GO TO 472
C
C     DEW TEMPERATURE CALCULATION APPLYING RAOULT'S LAW
C
  471 SUMX=0.0
      DO 442 I=1,NN
      CX(I)=Y(I)*P/PS(I)
  442 SUMX=SUMX+CX(I)
C
  472 IF(J.EQ.2)GO TO 147
      FO=ALOG(SUMX)
      GO TO 149
  147 F1=ALOG(SUMX)
  149 CONTINUE
      DO 6 I=1,NN
      X(I)=CX(I)/SUMX
    6 CONTINUE
C
      WRITE(1,*) IN,' SUMX= ',SUMX,'    T= ',T
      IF(IN.GT.250)          GO TO 107
      IF(ABS(F1).LE.EPS)  GO TO 109
      T=T-F1/(F1-F0)
      T=T-1.
      IF(T.LT.TLL.OR.T.GT.700) GO TO 414
      GO TO 100
  107 PRINT*,' NO SOLUTION FOR DEWT CALCULATION AT DATA    ',M
      NT=NT-1
      GO TO 212
C
C     PRINT OF THE RESULTS
C
  414 IF(IRP.EQ.1)GO TO 107
      IRP=1.0
      T=300.
      GO TO 100
C
  109 WRITE(1,*) 'TEMPERATURE= ',T
      DO 686  I=1,NN,2
  686 WRITE(1,*)'X(',I,')= ',X(I),' X(',I+1,')= ',X(I+1)
      IF(LFD.NE.3) GO TO 127
      DO 465 I=1,NN
      FHI(I)=1.0
  465 GAMA(I)=1.0
  127 DO 296 I=1,NN
      IF(XE(I).EQ.0.0) GO TO 236
  296 SED(I)=SED(I)+ABS(X(I)-XE(I))
```

```
  236 IF(TE(M).EQ.0.0) GO TO 237
      ET=ABS(TE(M)-T)
      SET=SET+ET
  237 DO 12 I=1,NN
      IF(XE(I).EQ.0) GO TO 235
   12 EX(I)=(X(I)-XE(I))/XE(I)*100
  235 DO 24 I=1,NN
      IF(I.NE.1) GO TO 22
      WRITE(6,1005) M,I,Y(I),XE(I),TE(M),T,GAMA(I),FHI(I),X(I),EX(I)
      GO TO 24
   22 WRITE(6,1006) I,Y(I),XE(I),GAMA(I),FHI(I),X(I),EX(I)
   24 CONTINUE
 1000 FORMAT(12X,I2,'.',1X,A20)
 1001 FORMAT(/,4X,'PRESSURE=  ',F6.3,' ATM',//,17X,'GIVEN',33X,'CALCULATED'
     + ,/,11X,20('-'),3X,42('-'),/,'DATA',1X,'COMP',4X,
     + 'Y',5X,'XE',6X,'TE',7X,'T',9X,'GAMA',6X,'FHI',8X,'X',8X,'E%',/,79('*
 1005 FORMAT(1X,I2,2X,I2,2X,F6.4,1X,F6.4,2X,F7.2,2X,F7.2,2X,F9.4,2X,F7.4
     +      ,3X,F6.4,3X,F6.2)
 1006 FORMAT(5X,I2,2X,F6.4,1X,F6.4,20X,F9.4,2X,F7.4,3X,F6.4,3X,F6.2)
  212 CONTINUE
      DO 396 I=1,NN
      IF(NN.EQ.2.AND.I.EQ.2)GO TO 452
      SED(I)=SED(I)/NT
      IF(SED(I).EQ.0.0) GO TO 452
  396 WRITE(6,1206) I,I,I,SED(I)
  452 IF(SET.EQ.0.0) GO TO 1256
      SET=SET/NT
      PRINT*,'THE NUMBER OF DATA POINTS= ',NT
      WRITE(6,1207) SET
 1206 FORMAT(/,15X,'ERROR ON X(',I1,')= ABS(X(',I1,')-XE(',I1,'))/'
     +,'DATA POINTS= ',F7.4,1H1)
 1207 FORMAT(/,15X,'ERROR ON T= ABS(TE-T)/DATA POINTS= ',F7.4,1H1)
 1256 RETURN
      END
C     ---------------------------------------------------
C
      SUBROUTINE DEWP(N,NN,ANTA,ANTB,ANTC,DEL,LFD,ZAR,RD,MU,IOD,COMP)
C
C     ---------------------------------------------------
      PARAMETER(K=9)
      PARAMETER(MMR=4)
      DIMENSION XU(K),XQ(K),GAMA(K),RQ(63,2),ZAR(K),VL(K),COMP(63)
      DIMENSION Y(K),XE(K),ANTA(K),ANTB(K),ANTC(K),HC(K),PE(100)
      DIMENSION YA(K,100),XEA(K,100),XQ0(K),YE(K),YEA(K,100)
      DIMENSION A(K),B(K),Z(K),APR(K),BPR(K),XA(K,100),X(K)
      DIMENSION FIL(K),EY(K),EX(K),VK(K),CX(K),PS(K),SED(K)
      COMMON/UNIQ/ R(K),Q(K),QP(K),PU(K,K)
      COMMON/UNIFAC1/RB(K,MMR),QB(K,MMR),TABLE(63,63),KONT(K)
      COMMON/UNIFAC2/ITAB(K,MMR),KQR(K,MMR),MNR(K)
      COMMON/CONV/ TC(K),PC(K),OMEGA(K)
      COMMON/FUGV/APRM,BPRM,APRIJ(K,K),FHI(K)
      COMMON/RFUGV/FHS(K)
      COMMON NAME(K),LFED,TYPE
      CHARACTER*6 COMP,CM1,TUI,PUI
      CHARACTER*20 NAME
      CHARACTER*9 LFED,TYPE
C
C     VAPOUR AND LIQUID DATA
C
      PRINT*,'PROGRAM STARTS ITERATION FOR DEWP CALCULATION'
      PRINT*,'*******************************************'
      EPS=0.000001
      DO 56 I=1,NN
   56 WRITE(1,1)NAME(I)
      WRITE(1,1)LFED
      WRITE(1,*)
```

```
      IF(RD.EQ.1) GO TO 177
      PRINT*,'ENTER TEMPERATURE(IN K OR C OR F)'
      READ(*,*) T
      PRINT*,'ENTER THE UNIT OF THE TEMPERATURE( K OR C OR F)'
      READ(*,1)TUI
      IF(TUI.EQ.'C')T=T+273.15
      IF(TUI.EQ.'F')T=(T+459.67)/1.8
      PRINT*,T,' K'
    1 FORMAT(A)
  177 CALL OUT(NN,0,COMP)
      WRITE(6,1001) T
      SEP=0.0
      DO 315 I=1,NN
  315 SED(I)=0.0
      DO 212 M=1,N
      SUMXX=0.0
      SUMYY=0.0
      IF(RD.EQ.1) GO TO 155
      DO 112 I=1,NN-1
      PRINT*,'ENTER VAPOUR MOLE FRACTION(Y) OF ',NAME(I),'AT DATA ',M
      READ(IOD,*) YA(I,M)
  112 PRINT*,YA(I,M)
      DO 114 I=1,NN-1
      PRINT*,'ENTER EXPERIMENTAL VALUE OF LIQUID MOLE FRACTION'
      PRINT*,'OF   ',NAME(I),'IF AVAILABLE,IF NOT ENTER 0'
      READ(IOD,*) XEA(I,M)
      PRINT*,XEA(I,M)
      IF(XEA(I,M).EQ.0)GO TO 155
  114 CONTINUE
      PRINT*,'ENTER EXPERIMENTAL VALUE OF PRESSURE (ATM OR MM HG)'
      PRINT*,'IF IT IS NOT AVAILABLE ENTER 0'
      PRINT*,'(PRESSURES FOR ALL DATA POINTS MUST HAVE SAME UNIT)'
      READ(IOD,*) PE(M)
      IF(M.GT.1)GO TO 123
      PRINT*,'ENTER UNIT OF THE PRESSURE(ATM OR MM HG)'
      READ(IOD,1)PUI
  123 IF(PUI.EQ.'MM HG')PE(M)=PE(M)/760
      PRINT*,PE(M),' ATM'
  155 DO 139 I=1,NN-1
      Y(I)=YA(I,M)
      XE(I)=XEA(I,M)
      SUMYY=SUMYY+Y(I)
      SUMXX=SUMXX+XE(I)
  139 CONTINUE
      Y(NN)=1.0-SUMYY
      XE(NN)=1.0-SUMXX
      IF(XEA(1,M).EQ.0.0)XE(NN)=0.0
C
C     ITERATION FOR DEWP CALCULATION
C
      IF(LFD.EQ.3) GO TO 471
      DO 2 I=1,NN
      X(I)=Y(I)
    2 CONTINUE
      P=1.0
      CR=82.057
      RT=82.057*T
      CALL VAPS(ANTA,ANTB,ANTC,T,PS,NN)
      CALL CONST(A,B,APR,BPR,NN,T,P,CR,PS,ANTA,ANTB,ANTC)
      CALL LMV(PC,TC,ZAR,VL,T,NN)
      CALL RFUGAC(Z,A,B,NN,T)
      IN=0
  100 IN=IN+1
      WRITE(1,*) IN,' SUMX= ',SUMX,' P= ',P
      SUMX=0.0
```

```
      [illegible]
      GO TO(72,73),LFD
   72 CALL UNIQUAC(X,T,NN,GAMA,HC)
      GO TO 75
   73 CALL UNIFAC(X,NN,T,GAMA,MU)
   75 DO 5 I=1,NN
      PCL=EXP(VL(I)*(P-PS(I))/RT)
      FIY=FHI(I)*P
      FILMP=GAMA(I)*PS(I)*FHS(I)*PCL
      IF(T/TC(I).GE.1.8) FILMP=HC(I)
      VK(I)=FILMP/FIY
      CX(I)=Y(I)/VK(I)
      SUMX=SUMX+CX(I)
    5 CONTINUE
      DO 6 I=1,NN
      X(I)=CX(I)/SUMX
    6 CONTINUE
      DF=SUMX-1.000
      IF(ABS(DF).LT.EPS) GO TO 109
      IF(IN.GT.250)      GO TO 107
      P=P/SUMX
      GO TO 100
  107 PRINT*,' NO SOLUTION FOR DEW PRESSURE CALCULATION AT DATA ',M
      NT=NT-1
      GO TO 212
C
C     DEW PRESSURE CALCULATION APPLYING RAOULT'S LAW
C
  471 P=0.0
      CALL VAPS(ANTA,ANTB,ANTC,T,PS,NN)
      DO 441 I=1,NN
  441 PT=PT+Y(I)/PS(I)
      P=1/PT
      DO 442 I=1,NN
      X(I)=P*Y(I)/PS(I)
      GAMA(I)=1.0
  442 FHI(I)=1.0
C
C     PRINT OF THE RESULTS
C
  109 WRITE(1,*)'PRESSURE= ',P
      DO 686 I=1,NN,2
  686 WRITE(1,*)'X(',I,')= ',X(I),' X(',I+1,')= ',X(I+1)
      IF(PE(M).EQ.0.0) GO TO 316
      SEP=SEP+ABS(P-PE(M))
  316 DO 319 I=1,NN
      IF(XE(I).EQ.0.0)GO TO 235
      SED(I)=SED(I)+ABS(X(I)-XE(I))
  319 EX(I)=(X(I)-XE(I))/XE(I)*100
  235 DO 24 I=1,NN
      IF(I.NE.1) GO TO 22
      WRITE(6,1005) M,I,Y(I),XE(I),PE(M),P,GAMA(I),FHI(I),X(I),EX(I)
      GO TO 24
   22 WRITE(6,1006) I,Y(I),XE(I),GAMA(I),FHI(I),X(I),EX(I)
   24 CONTINUE
 1000 FORMAT(12X,I2,'.',1X,A20)
 1001 FORMAT(/,4X,'TEMPERATURE=',F7.2,' K',//,17X,'GIVEN',33X,'CALCULATED'
    + ,/,11X,20('-'),3X,42('-'),/,'DATA',1X,'COMP',4X,
    + 'Y',5X,'XE',6X,'PE',7X,'P',9X,'GAMA',6X,'FHI',6X,'X',8X,'E%',/,79('*
 1005 FORMAT(1X,I2,2X,I2,2X,F6.4,1X,F6.4,2X,F7.3,2X,F7.3,2X,F9.4,2X,F7.4
    +      ,3X,F6.4,3X,F6.2)
 1006 FORMAT(5X,I2,2X,F6.4,1X,F6.4,20X,F9.4,2X,F7.4,3X,F6.4,3X,F6.2)
  212 CONTINUE
      DO 322 I=1,NN
      IF(SED(I).EQ.0.0) GO TO 325
      IF(NN.EQ.2.AND.I.EQ.2) GO TO 325
```

```
      SED(I)=SED(I)/NT
  322 WRITE(6,1111) I,I,I,SED(I)
  325 SEP=SEP/NT
      IF(SEP.EQ.0.0) GO TO 1256
      PRINT*,'NUMBER OF DATA POINTS=',NT
      WRITE(6,1112) SEP
 1111 FORMAT(/,10X,'ERROR ON X(',I1,')= ABS(XE(',I1,')-X(',I1,'))/'
     +,'DATA POINTS= ',F7.4)
 1112 FORMAT(/,10X,'ERROR ON PRESSURE= ABS(PE-P)/DATA POINTS= ',F7.4)
 1256 RETURN
      END
C     -----------------------------------------------------------------
C
      SUBROUTINE BUBP(N,NN,ANTA,ANTB,ANTC,DEL,LFD,ZAR,RD,MJ,IOD,COMP)
C
C     -----------------------------------------------------------------
      PARAMETER(K=9)
      PARAMETER(MMR=4)
      DIMENSION XU(K),XQ(K),GAMA(K),RQ(63,2),ZAR(K),VL(K),COMP(63)
      DIMENSION Y(K),XE(K),ANTA(K),ANTB(K),ANTC(K),HC(K),PE(100)
      DIMENSION YA(K,100),XEA(K,100),XQO(K),YE(K),YEA(K,100),X(K)
      DIMENSION A(K),B(K),Z(K),APR(K),BPR(K),XA(K,100),PS(K)
      DIMENSION FILMP(K),FIL(K),EY(K),CY(K),VK(K),DEL(K,K),SED(K)
      COMMON/UNIQ/ R(K),Q(K),QP(K),PU(K,K)
      COMMON/UNIFAC1/RB(K,MMR),QB(K,MMR),TABLE(63,63),KONT(K)
      COMMON/UNIFAC2/ITAB(K,MMR),KQR(K,MMR),MNR(K)
      COMMON/CONV/ TC(K),PC(K),OMEGA(K)
      COMMON/FUGV/APRM,BPRM,APRIJ(K,K),FHI(K)
      COMMON/RFUGV/FHS(K)
      COMMON NAME(K),LFED,TYPE
      CHARACTER*6 COMP,CM1,TUI,PUI
      CHARACTER*20 NAME
      CHARACTER*9 LFED,TYPE
C
C     VAPOR AND LIQUID  DATA
C
      PRINT*,'PROGRAM STARTS ITERATION FOR BUBBLEP CALCULATION'
      PRINT*,'*************************************************'
      EPS=0.0000001
      DO 56 I=1,NN
   56 WRITE(1,1)NAME(I)
      WRITE(1,1)LFED
      NT=N
      IF(RD.EQ.1)GO TO 177
      PRINT*,'ENTER TEMPERATURE(IN K OR F OR C)'
      READ(*,*) T
      PRINT*,'ENTER UNIT OF THE TEMPERATURE (K OR F OR C)'
      READ(*,1) TUI
      IF(TUI.EQ.'C')T=T+273.15
      IF(TUI.EQ.'F')T=(T+459.67)/1.8
      PRINT*,T,' K'
    1 FORMAT(A)
  177 CALL OUT(NN,0,COMP)
      WRITE(6,1001) T
      SEP=0.0
      DO 388 I=1,NN
  388 SED(I)=0.0
      DO 212 M=1,N
      SUMXX=0.0
      SUMYY=0.0
      IF(RD.EQ.1)GO TO 155
      DO 112 I=1,NN-1
      PRINT*,'ENTER LIQUID MOLE FRACTION(X) OF ',NAME(I),'AT DATA ',M
      READ(IOD,*) XA(I,M)
  112 PRINT*,XA(I,M)
      DO 114 I=1,NN-1
```

```
      PRINT*,'ENTER EXPERIMENTAL VALUE OF VAPOUR MOLE FRACTION'
      PRINT*,'OF ',NAME(I),'IF AVAILABLE,IF NOT ENTER 0'
      READ(IOD,*) YEA(I,M)
      PRINT*,YEA(I,M)
      IF(YEA(I,M).EQ.0) GO TO 155
  114 CONTINUE
      PRINT*,'ENTER EXPERIMENTAL VALUE OF PRESSURE(IN ATM OR MM HG)'
      PRINT*,'IF IT IS NOT AVAILABLE ENTER 0'
      PRINT*,'(PRESSURES FOR ALL DATA POINTS MUST HAVE SAME UNIT)'
      READ(IOD,*) PE(M)
      IF(M.GT.1) GO TO 123
      PRINT*,'ENTER UNIT OF THE PRESSURE( ATM OR MM HG)'
      READ(IOD,1) PUI
  123 IF(PUI.EQ.'MM HG')PE(M)=PE(M)/760
      PRINT*,PE(M),' ATM'
  155 DO 139 I=1,NN-1
      X(I)=XA(I,M)
      YE(I)=YEA(I,M)
      SUMXX=SUMXX+X(I)
      SUMYY=SUMYY+YE(I)
  139 CONTINUE
      X(NN)=1.0-SUMXX
      YE(NN)=1.0-SUMYY
      IF(YEA(1,M).EQ.0)YE(NN)=0.0
C
C     ITERATION FOR THE BUBBLEP CALCULATION
C
      IF(LFD.EQ.3) GO TO 471
      P=1.000
      DO 2 I=1,NN
      Y(I)=X(I)
    2 CONTINUE
      CR=82.057
      RT=82.057*T
      CALL VAPS(ANTA,ANTB,ANTC,T,PS,NN)
      CALL CONST(A,B,APR,BPR,NN,T,P,CR,PS,ANTA,ANTB,ANTC )
      CALL LMV(PC,TC,ZAR,VL,T,NN)
      CALL RFUGAC(Z,A,B,NN,T)
      GO TO(72,73),LFD
   72 CALL UNIQUAC(X,T,NN,GAMA,HC)
      GO TO 75
   73 CALL UNIFAC(X,NN,T,GAMA,MU)
   75 DO 5 I=1,NN
      PCL=EXP(VL(I)*(P-PS(I))/RT)
      FILMP(I)= GAMA(I)*PS(I)*FHS(I)*PCL
    5 CONTINUE
      IN=0
  100 IN=IN+1
      SUMY=0.0
      CALL FUGAC(ZMIX,Y,APR,BPR,NN,T,P,CR,DEL)
      DO 6 I=1,NN
      IF(T/TC(I).GE.1.8) FILMP(I)=HC(I)
      VK(I)=FILMP(I)/(FHI(I)*P)
      CY(I)=X(I)*VK(I)
      SUMY=SUMY+CY(I)
    6 CONTINUE
      WRITE(1,*)IN, ' SUMY=',SUMY ,' P= ',P
      DO 7 I=1,NN
      Y(I)=CY(I)/SUMY
    7 CONTINUE
      DF=SUMY-1.000
      IF(ABS(DF).LT.EPS) GO TO 109
      IF(IN.GT.250)      GO TO 107
      P=P*SUMY
      GO TO 100
  107 PRINT*,'NO SOLUTION FOR BUBBLEP CALCULATION AT DATA ',M
```

```
      NT=NT-1
      GO TO 212
C
C     BUBBLE PRESSURE CALCULATION USING RAOULT'S LAW
C
  471 P=0.0
      CALL VAPS(ANTA,ANTB,ANTC,T,PS,NN)
      DO 441 I=1,NN
  441 P=P+PS(I)*X(I)
      DO 442 I=1,NN
      Y(I)=X(I)*PS(I)/P
      GAMA(I)=1.0
  442 FHI(I)=1.0
C
C     PRINT  OF THE  RESULTS
C
  109 WRITE(1,*)'PRESSURE= ',P
      DO 686 I=1,NN,2
  685 WRITE(1,*)'Y(',I,')= ',Y(I),' Y(',I+1,')= ',Y(I+1)
      IF(PE(M).EQ.0.0)GO TO 398
      SEP=SEP+ABS(PE(M)-P)
 398  DO 397 I=1,NN
      IF(YE(I).EQ.0.0) GO TO 235
      SED(I)=SED(I)+ABS(YE(I)-Y(I))
 397  EY(I)=((Y(I)-YE(I))/YE(I))*100
 235  DO 24 I=1,NN
      IF(I.NE.1) GO TO 22
      WRITE(6,1005)M,I,X(I),YE(I),PE(M),P,GAMA(I),Y(I),FHI(I),EY(I)
      GO TO 24
 22   WRITE(6,1006)I,X(I),YE(I),GAMA(I),Y(I),FHI(I),EY(I)
 24   CONTINUE
 4212 CONTINUE
 1000 FORMAT(12X,I2,'.',1X,A20)
 1001 FORMAT(/,4X,'TEMPERATURE= ',F7.2,' K',//,17X,'GIVEN',33X,'CALCULATED'
     +  ,/,11X,20('-'),3X,42('-'),/,'DATA',1X,'COMP',4X,
     +  'X',5X,'YE',6X,'PE',7X,'P',9X,'GAMA',6X,'FHI',6X,'Y',8X,'E%',/,79('
 1005 FORMAT(1X,I2,2X,I2,2X,F6.4,1X,F6.4,2X,F7.3,2X,F7.3,2X,F9.4,2X,F7.4
     +      ,3X,F6.4,3X,F6.2)
 1005 FORMAT(5X,I2,2X,F6.4,1X,F6.4,20X,F9.4,2X,F7.4,3X,F6.4,3X,F6.2)
  212 CONTINUE
      DO 385 I=1,NN
      IF(SED(I).EQ.0.0)GO TO 376
      IF(I.EQ.2.AND.NN.EQ.2) GO TO 376
      SED(I)=SED(I)/NT
  385 WRITE(6,1111) I,I,I,SED(I)
  375 IF(SEP.EQ.0.0)GO TO 1256
      SEP=SEP/NT
      PRINT*,'NUMBER OF DATA POINTS=',NT
      WRITE(6,1112) SEP
 1111 FORMAT(/,10X,'ERROR ON Y(',I1,')= ABS(YE(',I1,')-Y(',I1,')/DATA'
     +,' POINTS= ',F7.4)
 1112 FORMAT(/,10X,'ERROR ON P= ABS(PE-P)/DATA POINTS=  ',F7.4,1H0)
 1255 RETURN
      END
C     -----------------------------------------------------------
C
      SUBROUTINE BUBT(N,NN,ANTA,ANTB,ANTC,DEL,LFD,ZAR,RD,MU,IOD,COMP)
C
C     ------------------------------------------------------------
      PARAMETER(K=9)
      PARAMETER(MMR=4)
      DIMENSION XU(K),XQ(K),GAMA(K),RQ(63,2),ZAR(K),VL(K),COMP(63)
      DIMENSION Y(K),XE(K),ANTA(K),ANTB(K),ANTC(K),HC(K),TE(100)
      DIMENSION YA(K,100),XEA(K,100),XQO(K),YE(K),YEA(K,100),X(K)
      DIMENSION A(K),B(K),Z(K),APR(K),BPR(K),XA(K,100)
      DIMENSION EY(K),CY(K),VK(K),DEL(K),PS(K),SED(K)
```

```
      COMMON/UNIQ/ R(K),Q(K),QP(K),PJ(K,K)
      COMMON/UNIFAC1/RB(K,MMR),QB(K,MMR),TABLE(63,63),KONT(K)
      COMMON/UNIFAC2/ITAB(K,MMR),KQR(K,MMR),MNR(K)
      COMMON/CONV/ TC(K),PC(K),OMEGA(K)
      COMMON/FUGV/APRM,BPRM,APRIJ(K,K),FHI(K)
      COMMON/RFUGV/FHS(K)
      COMMON NAME(K),LFED,TYPE
      CHARACTER*6 COMP,CM1,TUI,PUI
      CHARACTER*20 NAME
      CHARACTER*9  LFED,TYPE
C
C
C     ***************************************************************
      PRINT*,'PROGRAM STARTS ITERATION FOR BUBBLET CALCULATION'
      PRINT*,'***************************************************'
      EPS=0.00001
      DO 56 I=1,NN
   56 WRITE(1,1)NAME(I)
      WRITE(1,1)LFED
      NT=N
      IF(RD.EQ.1)GO TO 177
      PRINT*,'ENTER PRESSURE(IN ATM OR MM HG)'
      READ(*,*)P
      PRINT*,'ENTER UNIT OF THE PRESSURE( ATM OR MM HG)'
      READ(*,1)PUI
      IF(PUI.EQ.'MM HG')P=P/760
      PRINT*,P,' ATM'
    1 FORMAT(A)
  177 CALL OUT(NN,0,COMP)
      WRITE(6,1001) P
      SET=0.0
      DO 388 I=1,NN
  388 SED(I)=0.0
      DO 212 M=1,N
      SUMXX=0.
      SUMYY=0.
      IF(RD.EQ.1) GO TO 155
      DO 112 I=1,NN-1
      PRINT*,'ENTER LIQUID MOLE FRACTION(X) OF ',NAME(I),'AT DATA ',M
      READ(IOD,*) XA(I,M)
  112 PRINT*,XA(I,M)
      DO 114 I=1,NN-1
      PRINT*,'ENTER EXPERIMENTAL VALUE OF VAPOUR MOLE FRACTION'
      PRINT*,'OF ',NAME(I),'IF AVAILABLE,IF NOT ENTER 0'
      READ(IOD,*) YEA(I,M)
      PRINT*,YEA(I,M)
      IF(YEA(I,M).EQ.0) GO TO 155
  114 CONTINUE
      PRINT*,'ENTER EXPERIMENTAL VALUE OF TEMPERATURE(IN K OR C OR F)'
      PRINT*,'IF IT IS NOT AVAILABLE ENTER 0'
      PRINT*,'(TEMPERATURES FOR ALL DATA POINTS MUST HAVE SAME UNIT)'
      READ(IOD,*) TE(M)
      IF(TE(M).EQ.0.0)GO TO 155
      IF(M.GT.1)GO TO 123
      PRINT*,'ENTER UNIT OF THE TEMPERATURE( K OR F OR C)'
      READ(IOD,1) TUI
  123 IF(TUI.EQ.'C')TE(M)=TE(M)+273.15
      IF(TUI.EQ.'F')TE(M)=(TE(M)+459.67)/1.8
      PRINT*,TE(M),' K'
  155 DO 139 I=1,NN-1
      X(I)=XA(I,M)
      YE(I)=YEA(I,M)
      SUMXX=SUMXX+X(I)
      SUMYY=SUMYY+YE(I)
  139 CONTINUE
      X(NN)=1.0-SUMXX
```

```
      IF(YEA(1,M).EQ.0.0)YE(NN)=0.0
C
C     ITERATION PART FOR THE BUBBLET  CALCULATION
C
      IRP=0
      T=400
      DO 2 I=1,NN
      Y(I)=X(I)
  2   CONTINUE
      TLL=100.
      NNN=2
      IN=0
      CR=82.057
 100  IN=IN+1
      RT=82.057*T
 101  DO 149 J=1,NNN
      IF(J.EQ.2)T=T+1.
      CALL VAPS(ANTA,ANTB,ANTC,T,PS,NN)
      IF(LFD.EQ.3) GO TO 471
      CALL CONST(A,B,APR,BPR,NN,T,P,CR,PS,ANTA,ANTB,ANTC)
      CALL LMV(PC,TC,ZAR,VL,T,NN)
      CALL RFUGAC(Z,A,B,NN,T)
      GO TO (72,73),LFD
  72  CALL UNIQUAC(X,T,NN,GAMA,HC)
      GO TO 75
  73  CALL UNIFAC(X,NN,T,GAMA,MU)
  75  CALL FUGAC(ZMIX,Y,APR,BPR,NN,T,P,CR,DEL)
      SUMY=0
      DO 5 I=1,NN
      PCL=EXP(VL(I)*(P-PS(I))/RT)
      FIY=FHI(I)*P
      FILMP=GAMA(I)*PS(I)*FHS(I)*PCL
      IF(T/TC(I).GE.1.8) FILMP=HC(I)
      IF(T/TC(I).GE.1.8) TLL=0.0
      VK(I)=FILMP/FIY
      CY(I)=VK(I)*X(I)
      SUMY=SUMY+CY(I)
    5 CONTINUE
      IF(SUMY.GT.10000.OR.SUMY.LT.0.00001)GO TO 414
      GO TO 472
C
C     BUBBLE TEMPERATURE CALCULATION USING RAOULT'S LAW
C
  471 SUMY=0.0
      DO 442 I=1,NN
      CY(I)=X(I)*PS(I)/P
  442 SUMY=SUMY+CY(I)
C
  472 IF(J.EQ.2) GO TO 147
      F0=ALOG(SUMY)
      GO TO 149
  147 F1=ALOG(SUMY)
  149 CONTINUE
      DO 6 I=1,NN
      Y(I)=CY(I)/SUMY
   6  CONTINUE
      WRITE(1,*)IN,' SUMY= ',SUMY,' T= ',T
      IF(IN.EQ.250)      GO TO 107
      IF(ABS(F1).LE.EPS)GO TO 109
      T=T-F1/(F1-F0)
      T=T-1
      PRINT*,'T= ',T
      IF(T.LE.LTT.OR.T.GT.700.)GO TO 414
      GO TO 100
  107 PRINT*,'NO SOLUTION FOR BUBBLET CALCULATION AT DATA ',M
```

```
      NI=NI-1
      GO TO 212
C
  414 IF(IRP.EQ.1)GO TO 107
      IRP=1
      T=300.
      GO TO 100
C
C     PRINT  OF THE  RESULTS
C
  107 WRITE(1,*)'TEMPERATURE= ',T
      DO 686 I=1,NN,2
  686 WRITE(1,*)'Y(',I,')= ',Y(I),' Y(',I+1,')= ',Y(I+1)
      IF(LFD.NE.3) GO TO 457
      DO 568 I=1,NN
      GAMA(I)=1.0
  568 FHI(I)=1.0
  457 IF(TE(M).EQ.0.0) GO TO 376
      SET=SET+ABS(TE(M)-T)
  376 DO 378 I=1,NN
      IF(YE(I).EQ.0.0) GO TO 235
      SED(I)=SED(I)+ABS(YE(I)-Y(I))
 378  EY(I)=((Y(I)-YE(I))/YE(I))*100
 235  DO 24 I=1,NN
      IF(I.NE.1) GO TO 22
      WRITE(6,1005)M,I,X(I),YE(I),TE(M),T,GAMA(I),FHI(I),Y(I),EY(I)
      GO TO 24
  22  WRITE(6,1006)I,X(I),YE(I),GAMA(I),FHI(I),Y(I),EY(I)
  24  CONTINUE
 4212 CONTINUE
 1000 FORMAT(12X,I2,'.',1X,A20)
 1001 FORMAT(/,2X,'PRESSURE= ',F7.3,'  ATM',//,17X,'GIVEN',33X,'CALCULATED'
     +  ,/,11X,20('-'),3X,42('-'),/,'DATA',1X,'COMP',4X,
     +  'X',5X,'YE',6X,'TE',7X,'T',9X,'GAMA',6X,'FHI',6X,'Y',8X,'E%',/,)
 1005 FORMAT(1X,I2,2X,I2,2X,F6.4,1X,F6.4,2X,F7.2,2X,F7.2,2X,F9.4,2X,F7.4
     +      ,3X,F6.4,3X,F6.2)
 1006 FORMAT(5X,I2,2X,F6.4,1X,F6.4,20X,F9.4,2X,F7.4,3X,F6.4,3X,F6.2)
  212 CONTINUE
      DO 366 I=1,NN
      IF(SED(I).EQ.0.0) GO TO 356
      IF(I.EQ.2.AND.NN.EQ.2) GO TO 356
      SED(I)=SED(I)/NT
  366 WRITE(6,1111) I,I,I,SED(I)
  356 IF(SET.EQ.0.0) GO TO 1256
      PRINT*,'NUMBER OF DATA POINTS=',NT
      SET=SET/NT
      WRITE(6,1112) SET
 1111 FORMAT(/,10X,'ERROR ON Y(',I1,')= ABS(Y(',I1,')-YE(',I1,'))/'
     +,'DATA POINTS= ',F7.4)
 1112 FORMAT(/,10X,'ERROR ON TEMPERATURE= ABS(T-TE)/DATA POINTS= ',
     +F7.4)
 1256 RETURN
      END
C     ------------------------------------------------------------
C
      SUBROUTINE UNIQUAC(X,T,NN,GAM,HC)
C
C     ------------------------------------------------------------
      PARAMETER(M=9)
      DIMENSION X(M),GAM(M),RX(M),QX(M),HC(M),GAMN(M,M)
      DIMENSION QPX(M),L(M),THP(M),TOIJ(M,M),FHN(M),TR(M)
      COMMON/UNIQ/ R(M),Q(M),QP(M),PU(M,M)
      COMMON/CONV/ TC(M),PC(M),OMEGA(M)
C
      REAL L,LX
      Z=10.
```

```
      DO 51 I=1,NN
   51 TR(I)=T/TC(I)
      DO 52 I=1,NN
      IF(TR(I).LT.1.8) GO TO 52
      R(I)=0.0
      Q(I)=0.0
      QP(I)=0.0
   52 CONTINUE
      SUMRX=0.0
      SUMQX=0.0
      SUMQPX=0.0
      SUMLX=0.0
      DO 11 I=1,NN
      IF(X(I).EQ.0.0) GO TO 11
      RX(I)=R(I)*X(I)
      QX(I)=Q(I)*X(I)
      QPX(I)=QP(I)*X(I)
      L(I)=(Z/2.)*(R(I)-Q(I))-(R(I)-1.)
      LX=L(I)*X(I)
      SUMRX=SUMRX+RX(I)
      SUMQX=SUMQX+QX(I)
      SUMQPX=SUMQPX+QPX(I)
      SUMLX=SUMLX+LX
   11 CONTINUE
      DO 21 I=1,NN
      IF(X(I).EQ.0.0) GO TO 21
      THP(I)=QPX(I)/SUMQPX
   21 CONTINUE
      DO 14 I=1,NN
      DO 15 J=1,NN
      IF(I.EQ.J) GO TO 75
      IF(TR(I).GE.1.8.OR.TR(J).GE.1.8) GO TO 75
      TOIJ(J,I)=EXP(-PU(J,I)/T)
      GO TO 15
   75 TOIJ(J,L)=1.0
   15 CONTINUE
   14 CONTINUE
      DO 22 I=1,NN
      IF(TR(I).GE.1.8) GO TO 55
      SUM1=0.0
      DO 23 J=1,NN
      TOTP1=TOIJ(J,I)*THP(J)
      SUM1=SUM1+TOTP1
   23 CONTINUE
      SUM3=0.0
      DO 24 J=1,NN
      SUM2=0.0
      DO 25 K=1,NN
      TOTP2=TOIJ(K,J)*THP(K)
      SUM2=SUM2+TOTP2
   25 CONTINUE
      TOTP3=TOIJ(I,J)*THP(J)
      TT3OS=TOTP3/SUM2
      SUM3=SUM3+TT3OS
   24 CONTINUE
      TH=QX(I)/SUMQX
      PH=RX(I)/SUMRX
      A1=ALOG(PH/X(I))
      A2=(Z/2)*Q(I)*ALOG(TH/PH)
      A3=PH*SUMLX/X(I)
      A4= QP(I)*ALOG(SUM1)
      A5=QP(I)*SUM3
      GAME=A1+A2+L(I)-A3-A4+QP(I)-A5
      GAM(I)=EXP(GAME)
      GO TO 22
C
```

```
C     ACTIVITY COEFFICIENTS OF NONCONDENSABLE COMPONENTS  ARE CALCULATED
C
   55 SUMGAM=0.0
      SUMFH=0.0
      CALL RFUGNC(T,TC(I),PC(I),FHN(I))
      DO 61 JS=1,NN
      IF(TR(JS).GT.1.8) GO TO 61
      GAMN(I,JS)=PU(I,JS)+(PU(JS,I)/T)
      TH=QX(JS)/SUMQX
      SUMGAM=SUMGAM+GAMN(I,JS)*TH
      SUMFH=SUMFH+TH
   61 CONTINUE
      HC(I)=SUMGAM+SUMFH*ALOG(FHN(I))
      HC(I)=EXP(HC(I))
      GAM(I)=EXP(SUMGAM)
   22 CONTINUE
      RETURN
      END
C     ------------------------------------------------------------------
C
      SUBROUTINE UNIFAC (XLIQ,NN,T,GAMA,MU)
C
C     ------------------------------------------------------------------
      PARAMETER (K=9)
      PARAMETER (MMR=4)
      DIMENSION XLIQ(K),RLT(K),QLT(K),SUMTD(K),OME(K)
      DIMENSION TETA(K),PHIC(K),EL(K),GCLN(K),TETAD(K,MMR),TETAN(K,MMR)
      DIMENSION CONTR(K,K,MMR,MMR),PSI(K,K,MMR,MMR),SUMO2(MMR)
      DIMENSION SUMO(K,MMR),ODDLN(K,MMR),SUMO3(K,MMR),XBIG(K,MMR)
      DIMENSION TETARM(K,MMR),SUMON5(K,MMR),SUMOM1(K,MMR),SUMOM4(K,MMR)
      DIMENSION ODLN(K,MMR),GRLN(K),GAMA(K)
      COMMON/UNIFAC1/RB(K,MMR),QB(K,MMR),TABLE(63,63),KONT(K)
      COMMON/UNIFAC2/ITAB(K,MMR),KQR(K,MMR),MNR(K)
C
      DO 1 I=1,NN
      SUMR=0
      SUMQ=0
      J=1
   30 SUMR=SUMR+RB(I,J)*KQR(I,J)
      SUMQ=SUMQ+QB(I,J)*KQR(I,J)
      IF (J.EQ.KONT(I)) GO TO 20
      J=J+1
      GO TO 30
   20 RLT(I)=SUMR
      QLT(I)=SUMQ
    1 CONTINUE
      SUMRX=0
      SUMQX=0
      SUMMR=0
      PME=2/3
      DO 3 I=1,NN
      SUMRX=SUMRX+XLIQ(I)*RLT(I)
      SUMQX=SUMQX+XLIQ(I)*QLT(I)
      SUMMR=SUMMR+XLIQ(I)*(RLT(I)**PME)
    3 CONTINUE
      IF(MU.EQ.1) GO TO 177
      DO 4 I=1,NN
      TETA(I)=XLIQ(I)*QLT(I)/SUMQX
      PHIC(I)=XLIQ(I)*RLT(I)/SUMRX
      EL(I)=5*(RLT(I)-QLT(I))-(RLT(I)-1.0)
    4 CONTINUE
      SUML=0
      DO 5 I=1,NN
      SUML=SUML+XLIQ(I)*EL(I)
    5 CONTINUE
      DO 6 I=1,NN
```

```
      GC1=ALOG(PHIC(I)/XLIQ(I))
      GC2=5*QLT(I)*ALOG(TETA(I)/PHIC(I))
      GC3=EL(I)-SUML*PHIC(I)/XLIQ(I)
      GCLN(I)=GC1+GC2+GC3
    5 CONTINUE
      GO TO 178
C
C     FOR THE COMBINATORIAL PART MODIFIED UNIFAC APPLIED
C
  177 DO 235 I=1,NN
      OME(I)=XLIQ(I)*(RLT(I)**PME)/SUMMR
      GCLN(I)=ALOG(OME(I)/XLIQ(I))+1-OME(I)/XLIQ(I)
  235 CONTINUE
C
  178 DO 666 I=1,NN
      SUMTD(I)=0
  666 CONTINUE
      DO 7 I=1,NN
      DO 15 J=1,KONT(I)
      TETAD(I,J)=KQR(I,J)*QB(I,J)/MNR(I)
      SUMTD(I)=SUMTD(I)+TETAD(I,J)
   15 CONTINUE
    7 CONTINUE
      DO 8 I=1,NN
      DO 14 J=1,KONT(I)
      TETAN(I,J)=TETAD(I,J)/SUMTD(I)
   14 CONTINUE
    8 CONTINUE
      DO 9 I=1,NN
      DO 12 J=1,NN
      DO 16 M=1,KONT(I)
      DO 49 N=1,KONT(J)
      ITB=ITAB(I,M)
      ITA=ITAB(J,N)
C     IF(MU.EQ.0)GO TO 179
C     TABLE(ITB,ITA)=TABLE(ITB,ITA)+TABLE(ITB,ITA)*(T-298.15)+
C     TABLE(ITB,ITA)*(T*ALOG(298.15/T)+T-298.15)
      CONTR(I,J,M,N)=TABLE(ITB,ITA)
      PSI(I,J,M,N)=EXP(0-CONTR(I,J,M,N)/T)
   49 CONTINUE
   16 CONTINUE
   12 CONTINUE
    9 CONTINUE
      KK=MMR
      DO 56 I=1,NN
      DO 57 II=1,KK
      SUMO2(II)=0
   57 CONTINUE
      MM=1
      DO 55 J=1,KONT(I)
      SUMOD1=0
      DO 54 N=1,KONT(I)
      SUMOD1=SUMOD1+TETAN(I,N)*PSI(I,I,N,MM)
   54 CONTINUE
      SUMO3(I,J)=SUMOD1
      DO 52 JJ=1,KONT(I)
      SUMTR=TETAN(I,J)*PSI(I,I,JJ,MM)/SUMO3(I,J)
      SUMO(I,JJ)=SUMO2(JJ)+SUMTR
      SUMO2(JJ)=SUMO(I,JJ)
   52 CONTINUE
      MM=MM+1
   55 CONTINUE
   56 CONTINUE
      DO 58 I=1,NN
      DO 59 J=1,KONT(I)
      ODDLN(I,J)=QB(I,J)*(1-ALOG(SUMO3(I,J))-SUMO(I,J))
```

```
57    CONTINUE
58    CONTINUE
      SUMXB=0
      DO 67 I=1,NN
      XBIGD=SUMXB+XLIQ(I)*MNR(I)
      SUMXB=XBIGD
67    CONTINUE
      DO 61 I=1,NN
      DO 62 J=1,KONT(I)
      XBIGN=KQR(I,J)*XLIQ(I)
      DO 63 II=1,NN
      DO 64 JJ=1,KONT(II)
      IF((ITAB(I,J).EQ.ITAB(II,JJ)).AND.(I.NE.II)) GO TO 81
      GO TO 64
81    XBIGN=XBIGN+KQR(II,JJ)*XLIQ(II)
64    CONTINUE
63    CONTINUE
      XBIG(I,J)=XBIGN/XBIGD
62    CONTINUE
61    CONTINUE
      SUMT=0
      DO 17 I=1,NN
      DO 18 J=1,KONT(I)
      SUMT=SUMT+XBIG(I,J)*QB(I,J)
      DO 65 II=I,NN
      DO 66 JJ=1,KONT(II)
      ADT=XBIG(I,J)*QB(I,J)
      IF((ITAB(I,J).EQ.ITAB(II,JJ)).AND.(I.NE.II)) SUMT=SUMT-ADT
66    CONTINUE
65    CONTINUE
18    CONTINUE
17    CONTINUE
      DO 70 I=1,NN
      DO 71 J=1,KONT(I)
      TETARM(I,J)=XBIG(I,J)*QB(I,J)/SUMT
71    CONTINUE
70    CONTINUE
      DO 83 I=1,NN
      MM=1
      DO 82 J=1,KONT(I)
      SUMOD2=0
      DO 73 II=1,NN
      DO 72 JJ=1,KONT(II)
      SUMOD2=SUMOD2+TETARM(II,JJ)*PSI(II,I,JJ,MM)
      DO 21 I1=II,NN
      DO 22 J1=1,KONT(I1)
      SMNS=TETARM(I1,J1)*PSI(I1,I,J1,MM)
      IF((ITAB(I1,J1).EQ.ITAB(II,JJ)).AND.(I1.NE.II)) GO TO 91
      GO TO 22
91    SUMOD2=SUMOD2-SMNS
      GO TO 72
22    CONTINUE
21    CONTINUE
72    CONTINUE
73    CONTINUE
      SUMOM1(I,J)=SUMOD2
      MM=MM+1
82    CONTINUE
83    CONTINUE
      DO 78 I=1,NN
      DO 79 J=1,KONT(I)
      SUMON5(I,J)=0
79    CONTINUE
78    CONTINUE
      DO 76 I=1,NN
      MM=1
```

```
      SUMON7=0
      DO 23 II=1,NN
      DO 24 JJ=1,KONT(II)
      LO=1
      DO 25 III=II,NN
      DO 26 JJJ=1,KONT(III)
      IF((ITAB(II,JJ).EQ.ITAB(III,JJJ)).AND.(II.NE.III))LO=0
   26 CONTINUE
   25 CONTINUE
      SUMF=TETARM(II,JJ)*PSI(I,II,MM,JJ)*LO
      SUMON7=SUMON7+SUMF/SUMOM1(II,JJ)
      SUMOM4(I,J)=SUMON7
   24 CONTINUE
   23 CONTINUE
      MM=MM+1
   77 CONTINUE
   75 CONTINUE
      DO 84 I=1,NN
      DO 85 J=1,KONT(I)
      ODLN(I,J)=QB(I,J)*(1-ALOG(SUMOM1(I,J))-SUMOM4(I,J))
   85 CONTINUE
   84 CONTINUE
      DO 86 I=1,NN
      SUMG=0
      DO 87 J=1,KONT(I)
      GRLN(I)=KQR(I,J)*(ODLN(I,J)-ODDLN(I,J))+SUMG
      SUMG=GRLN(I)
   87 CONTINUE
   86 CONTINUE
      DO 89 I=1,NN
      GAMA(I)=EXP(GRLN(I)+GCLN(I))
   89 CONTINUE
      RETURN
      END
C
      FUNCTION FINDR (CM,COMP)
C
      CHARACTER*6 COMP(63),CM
      DO 10 I=1,63
      IF (COMP(I).EQ.CM) GO TO 20
   10 CONTINUE
      PRINT*,'ILLEGAL COMPOUND NAME _ ENTER AGAIN'
      FINDR=-1
      RETURN
   20 FINDR=I
      RETURN
      END
C     ------------------------------------------------------------
C
      SUBROUTINE CONST(A,B,APR,BPR,NN,T,P,R,PS,ANTA,ANTB,ANTC)
C
C     ------------------------------------------------------------
      PARAMETER(K=9)
      COMMON /CONV/ TC(K),PC(K),OMEGA(K)
      DIMENSION A(K),B(K),APR(K),BPR(K),PS(K)
      DIMENSION ANTA(K),ANTB(K),ANTC(K)
      REAL KAPA
      DO 292 I=1,NN
      IF(OMEGA(I).NE.0.0) GO TO 222
      OMEGA(I)=ACEF(ANTA(I),ANTB(I),ANTC(I),TC(I),PC(I))
  222 KAPA=0.37464+1.54226*OMEGA(I)-0.26992*OMEGA(I)**2
      TR=T/TC(I)
      ALPHA=(1+KAPA*(1-SQRT(TR)))**2
      ATC=0.45724*R*R*TC(I)*TC(I)/PC(I)
      APR(I)=ATC*ALPHA
```

```
      IF(TR.GE.1.8) GO TO 292
      A(I)=APR(I)*PS(I)/(R*R*T*T)
      B(I)=BPR(I)*PS(I)/(R*T)
  292 CONTINUE
      RETURN
      END
C     ----------------------------------------------------------------
C
      SUBROUTINE FUGAC(ZMIX,Y,APR,BPR,NN,T,P,R,DEL)
C
C     ----------------------------------------------------------------
      PARAMETER(K=9)
      COMMON /FUGV/ APRM,BPRM,APRIJ(K,K),FHI(K)
      DIMENSION Y(K),APR(K),BPR(K),DEL(K,K)
      DO 392 I=1,NN
      DO 492 J=1,NN
      APRIJ(I,J)=(1-DEL(I,J))*SQRT(APR(I)*APR(J))
  492 CONTINUE
  392 CONTINUE
      APRM=0
      DO 4392 I=1,NN
      DO 3392 J=1,NN
      YAIJ=Y(I)*Y(J)*APRIJ(I,J)
      APRM=APRM+YAIJ
 3392 CONTINUE
      BPRM=Y(I)*BPR(I)
 4392 CONTINUE
      AMIX=APRM*P/(R*R*T*T)
      BMIX=BPRM*P/(R*T)
      CALL ROOT(AMIX,BMIX,ZMIX)
      A1=(ZMIX-1)/BPRM
      A2= ALOG(ZMIX-BMIX)
      A4= AMIX/(2*1.41*BMIX)
      AK=(ZMIX+2.414*BMIX)/(ZMIX-0.41  *BMIX)
      A5= ALOG((ZMIX+2.414*BMIX)/(ZMIX-0.414*BMIX))
      DO 111 J=1,NN
      AY=0.0
      DO 112 I=1,NN
      AY=AY+Y(I)*APRIJ(I,J)
  112 CONTINUE
      A3=2*AY/APRM-BPR(J)/BPRM
      FHI(J)=EXP(BPR(J)*A1-A2-A4*A3*A5)
  111 CONTINUE
      RETURN
      END
C     ----------------------------------------------------------------
C
      SUBROUTINE RFUGAC(Z,A,B,NN,T)
C
C     ----------------------------------------------------------------
      PARAMETER(K=9)
      COMMON /RFUGV/ FHS(K)
      COMMON/CONV/TC(K),PC(K),OMEGA(K)
      DIMENSION Z(K),A(K),B(K)
      DO 155 I=1,NN
      IF(T/TC(I).GE.1.8) GO TO 155
      CALL ROOT(A(I),B(I),Z(I))
      A1=ALOG(Z(I)-B(I))
      A2=A(I)/(2*1.41*B(I))
      A3=ALOG((Z(I)+2.414*B(I))/(Z(I)-0.414*B(I)))
      FHS(I)=EXP(Z(I)-1-A1-A2*A3)
  155 CONTINUE
      RETURN
      END
C     ----------------------------------------------------------------
```

```
C
      SUBROUTINE ROOT(A,B,Z)
C
C     ----------------------------------------------------------------
      Z=1
      INN=1
  170 F=Z**3-(1-B)*Z**2+(A-3*B**2-2*B)*Z-(A*B-B**2-B**3)
      FD=3*Z**2-2*(1-B)*Z+(A-3*B**2-2*B)
      IF(INN.EQ.1) GO TO 150
      IF(ABS(Z-ZOLD).LT.0.00001) GO TO 160
  150 ZOLD=Z
      Z=Z-F/FD
      INN=INN+1
      GO TO 170
  160 RETURN
      END
C     -------------------------------------------------------------------
C
      SUBROUTINE VAPS(ANTA,ANTB,ANTC,T,PIS,NN)
C
C     -------------------------------------------------------------------
      PARAMETER(K=9)
      DIMENSION ANTA(K),ANTB(K),ANTC(K),PIS(K)
      COMMON/CONV/TC(K),PC(K),OMEGA(K)
      DO 76 I=1,NN
      IF(T/TC(I).GE.1.8) GO TO 76
      PIS(I)=EXP(ANTA(I)-ANTB(I)/(T+ANTC(I)))
      PIS(I)=PIS(I)/760
   76 CONTINUE
      RETURN
      END
C     -------------------------------------------------------------------
C
      SUBROUTINE LMV(PC,TC,ZAR,VL,T,NN)
C
C     -------------------------------------------------------------------
      PARAMETER(K=9)
      DIMENSION PC(K),TC(K),ZAR(K),VL(K)
      R=82.057
      DO 5  I=1,NN
      TR=T/TC(I)
      IF(TR.GT.0.75) GO TO 10
      TO=1+(1-TR)**(2./7.)
      GO TO 20
   10 TO=1.60+0.00693026/(TR-0.655)
   20 VL(I)=R*TC(I)*ZAR(I)**TO/PC(I)
    5 CONTINUE
      RETURN
      END
C
      FUNCTION ACEF(ANA,ANB,ANC,TK,PK)
C
      TW=0.7*TK
      PSW=EXP(ANA-ANB/(TW+ANC))
      PSW=PSW/760
      ACEF=-LOG(PSW/PK)-1.00
      RETURN
      END
C
C     -------------------------------------------------------------------
C
      SUBROUTINE OUT(NN,IPT,COMP)
C
C     -------------------------------------------------------------------
      PARAMETER (M=9,MMR=4)
      DIMENSION GSN(50),COMP(63)
```

```
      COMMON/UNIQ/ R(M),Q(M),QP(M),PJ(M,M)
      COMMON/UNIFAC1/RB(M,MMR),QB(M,MMR),TABLE(63,63),KONT(M)
      COMMON/UNIFAC2/ITAB(M,MMR),KQR(M,MMR),MNR(M)
      CHARACTER*20 NAME
      CHARACTER*9 LFED
      CHARACTER*6 TYPE,GROUP(50),COMP
C
      IF(IPT.EQ.1)GO TO 250
      WRITE(6,2222)
 2222 FORMAT(//,9X,'TABLE(     )          VLE CALCULATION RESULTS',/)
      K=NN/3
      IF(K.GT.(NN/3))K=K-1
      K=3*K
      EN=NN-K
  22  DO 5 I=1,K,3
   5  WRITE(6,1115) I,NAME(I),I+1,NAME(I+1),I+2,NAME(I+2)
      IF(K.EQ.NN) GO TO 15
      GO TO (10,11)EN
  10  WRITE(6,1125)NN,NAME(NN)
      GO TO 15
  11  WRITE(6,1126) NN-1,NAME(NN-1),NN,NAME(NN)
  15  WRITE(6,1116) TYPE
      IF(LFED.EQ.'RAOULT')GO TO 666
      WRITE(6,1117)LFED
      GO TO 919
  666 WRITE(6,1118)
      GO TO 919
 1115 FORMAT(4X,3(I2,'.',A20,1X))
 1125 FORMAT(4X,I2,'.',A20,1X)
 1126 FORMAT(4X,2(I2,'.',A20,1X))
 1116 FORMAT(/,10X,'TYPE: ',A4 )
 1117 FORMAT(/,10X,'LIQUID PHASE NONIDEALITY IS  CALCULATED BY '
     +,A8,' EQUATION',/,10X,'VAPOUR PHASE NONIDEALITY IS CALCULATED BY ',
     +'PENG ROBINSON EQUATION')
 1118 FORMAT(/,10X,'CALCULATIONS ARE PERFORMED BY RAOULT"S LAW')
  250 IF(LFED.EQ.'UNIFAC'.OR.LFED.EQ.'MODUNIFAC')GO TO 500
      WRITE(6,1000)
      DO 716 I=1,NN
  716 WRITE(6,1001) I,R(I),Q(I),QP(I)
      WRITE(6,1002)
      DO 717 I=1,NN-1
      DO 717 J=I+1,NN
  717 WRITE(6,1003)I,J,PJ(I,J),PU(J,I)
 1000 FORMAT(///,15X,'UNIQUAC PARAMETERS',//,10X,'COMP',5X,'R',
     +     8X,'Q',8X,'QP',/,9X,6('-'),4X,3('-'),6X,3('-'),6X,4('-'))
 1001 FORMAT(12X,I2,4X,F5.2,4X,F5.2,5X,F5.2)
 1002 FORMAT(//,16X,'COMPI',4X,'COMPJ',11X,'A(I,J)',9X,'A(J,I)',/,
     +15X,7('-'),2X,7('-'),9X,8('-'),7X,8('-'))
 1003 FORMAT(18X,I2,7X,I2,10X,F8.2,7X,F8.2)
      GO TO 929
  500 WRITE(6,1011) LFED
      ISI=0
      DO 726 I=1,NN
      DO 726 J=1,KONT(I)
      WRITE(6,1015) COMP(ITAB(I,J)),RB(I,J),QB(I,J)
      ISI=ISI+1
      GROUP(ISI)=COMP(ITAB(I,J))
  726 GSN(ISI)=ITAB(I,J)
      WRITE(6,1016)
      DO 727 I=1,ISI
      DO 727 J=I+1,ISI
      IF(GROUP(I).EQ.GROUP(J)) GO TO 727
      WRITE(6,1017) GROUP(I),GROUP(J),TABLE(GSN(I),GSN(J)),
     +     TABLE(GSN(J),GSN(I))
  727 CONTINUE
 1011 FORMAT(///,15X,A9,' PARAMETERS',//,15X,'GROUP',7X,'R',
```

```
     +      8X,'Q',/,14X,7('-'),5X,5('-'),6X,5('-'))
 1015 FORMAT(14X,A6,5X,F6.4,3X,F5.3)
 1015 FORMAT(//,15X,'GROUP',5X,'GROUP',5X,'A(I,J)',5X,'A(J,I)',/,
     +14X,7('-'),3X,7('-'),3X,8('-'),3X,8('-'))
 1017 FORMAT(14X,A6,4X,A6,4X,F8.2,3X,F8.2)
  929 WRITE(6,1256)
 1255 FORMAT(/,80('_'),/,80('-'))
  919 RETURN
      END
C     ------------------------------------------------------------------
C
      SUBROUTINE INPUT(ANTA,ANTB,ANTC,ZAR,DEL,LFD,NN,SCN,NRA,COMP)
C
C     ------------------------------------------------------------------
      PARAMETER (K=9,LKK=100)
      PARAMETER (MMR=4)
      DIMENSION RQ(63,2),NS(LKK),DEL(K,K),ZAR(K),COMP(63)
      DIMENSION ANTA(K),ANTB(K),ANTC(K)
      DIMENSION TCD(LKK),PCD(LKK),ATA(LKK),ATB(LKK),ATC(LKK)
      DIMENSION ZARD(LKK),DELD(10),OMEG(LKK)
      DIMENSION RD(LKK),QD(LKK),QPD(20),UU(LKK,LKK)
      COMMON/CONV/ TC(K),PC(K),OMEGA(K)
      COMMON/UNIQ/ R(K),Q(K),QP(K),PU(K,K)
      COMMON/UNIFAC1/RB(K,MMR),QB(K,MMR),TABLE(63,63),KONT(K)
      COMMON/UNIFAC2/ITAB(K,MMR),KQR(K,MMR),MNR(K)
      COMMON NAME(K),LFED,TYPE
      CHARACTER*6 COMP,CM1
      CHARACTER* 20 NAME,LFED,TYPE
      CHARACTER* 20 CODE(LKK),CODEP(20),ICODE(LKK),IJCODE(LKK,LKK)
      CHARACTER* 20 CODEPP(LKK),CODEDEL(10)
C
C     READS PHYSICAL PROPERTIES OF COMPONENTS
C
      IF(INPP.EQ.1) GO TO 389
      INPP=1
      CALL PF('GET','YDATAPP')
      READ(2,*) PP
      DO 201 I=1,PP
      READ(2,1) CODEPP(I)
      READ(2,*)TCD(I),PCD(I),ATA(I),ATB(I),ATC(I),ZARD(I),OMEG(I)
  201 CONTINUE
      DO 375 J=1,8
  375 READ(2,1200) CODEDEL(J),DELD(J)
 1200 FORMAT(A20,2X,F6.2)
  389 DO 345 I=1,NN
      DO 378 J=1,PP
      IF(NAME(I).EQ.CODEPP(J)) GO TO 388
  378 CONTINUE
      PRINT*,'TC,PC,ANTA,ANTB,ANTC,ZAR, ARE NOT AVAILABLE'
      PRINT*,'FOR THE ',NAME(I)
      READ*,TC(I),PC(I),ANTA(I),ANTB(I),ANTC(I),ZAR(I)
      GO TO 345
  388 TC(I)=TCD(J)
      PC(I)=PCD(J)
      ANTA(I)=ATA(J)
      ANTB(I)=ATB(J)
      ANTC(I)=ATC(J)
      ZAR(I)=ZARD(J)
      OMEGA(I)=OMEG(J)
  345 CONTINUE
C     DO 495 I=1,NN
C 495 PRINT*,'TC(',I,')= ',TC(I),' PC(',I,')= ',PC(I),' ZAR(',I,')= ',
CZAR(I)
      DO 595 I=1,NN
  595 IF(NAME(I).EQ.'WATER') GO TO 497
      GO TO 655
```

```
      DO 496 N=1,8
      IF(NAME(J).EQ.CODEDEL(N)) GO TO 475
  495 CONTINUE
      GO TO 501
  475 DEL(I,J)=DELD(N)
      PRINT*,'DEL= ',DEL(I,J)
  501 CONTINUE
  655 IF(LFD.EQ.2) GO TO 8
      IF(LFD.EQ.3) GO TO 919
C
C     UNIQUAC PARAMETERS ARE READ IN THIS SECTION
C
      IF(IUQ.EQ.1) GO TO 889
      IUQ=1
      CALL PF('GET','YDATAUQ')
      READ(3,*) NUP
      DO 181  I=1,NUP
 181  READ(3,1250) CODE(I),RD(I),QD(I)
 1250 FORMAT(2X,A20,1X,F5.2,2X,F4.2)
      READ(3,*)NUPE
      DO 182  I=1,NUPE
 182  READ(3,1252) CODEP(I),QPD(I)
 1252 FORMAT(2X,A20,2X,F4.2)
      READ(3,*) NUIP
      DO 183 I=1,NUIP
      READ(3,1) ICODE(I)
    1 FORMAT(A)
      READ(3,*)NS(I)
      DO 283 J=1,NS(I),2
      READ(3,1254) IJCODE(I,J),UU(I,J),IJCODE(I,J+1),UU(I,J+1)
  283 CONTINUE
 1254 FORMAT(A20,2X,F8.2,2X,A20,2X,F8.2)
 183  CONTINUE
 889  DO 185  I=1,NN
C     PRINT*,'NAME(',I,')=',NAME(I)
      DO 186  J=1,NUP
      IF(NAME(I).EQ.CODE(J)) GO TO 35
 186  CONTINUE
      GO TO 199
  35  R(I)=RD(J)
      Q(I)=QD(J)
      DO 187 KK=1,NUPE
      IF(NAME(I).EQ.CODEP(KK)) GO TO 36
 187  CONTINUE
      QP(I)=Q(I)
C     PRINT*,'R= ',R(I),' Q= ',Q(I),' QP= ',QP(I)
      GO TO 37
  36  QP(I)=QPD(KK)
  37  DO 188 J=1,NUIP
      IF(ICODE(J).EQ.NAME(I)) GO TO 39
 188  CONTINUE
  38  PRINT*,'INTERACTION PARAMETER OF COMPONENT ',NAME(I)
      PRINT*,'WITH OTHER COMPONENTS ARE NOT AVAILABLE'
      GO TO 200
  39  DO 191 KK=1,NN
      IF(NAME(KK).EQ.NAME(I)) GO TO 172
      DO 192 L=1,NS(J)
      IF(IJCODE(J,L).EQ.NAME(KK)) GO TO 42
  192 CONTINUE
      GO TO 38
  42  PU(I,KK)=UU(J,L)
C     PRINT*,'PU(',I,KK,')= ',PU(I,KK)
      GO TO 191
  172 PU(I,KK)=0.0
  191 CONTINUE
```

```
  180 CONTINUE
      GO TO 919
  199 PRINT*,'R AND Q PARAMETERS ARE NOT AVAILABLE FOR THE COMPONENT'
      PRINT*,NAME(I)
  200 PRINT*,'                         '
      PRINT*,'THE CALCULATION WILL BE PERFORMED BY UNIFAC EQUATION'
      LFD=2
C
C     DATA INPUT  FOR UNIFAC CALCULATION
C
    8 IF(NRA.EQ.1)GO TO 919
      IF(IUF.EQ.1)GO TO 875
      IUF=1
      CALL PF('GET','YDATUM')
      DO 99 I=1,63
      READ (UNIT=4,FMT=999,END=875) COMP(I),RQ(I,1),RQ(I,2)
  999 FORMAT (A6,2X,F6.4,2X,F5.3)
   99 CONTINUE
      DO 998 I=1,63
      READ (UNIT=4,FMT=997,END=875) (TABLE(I,J),J=1,10)
      READ (UNIT=4,FMT=997,END=875) (TABLE(I,J),J=11,20)
      READ (UNIT=4,FMT=997,END=875) (TABLE(I,J),J=21,30)
      READ (UNIT=4,FMT=997,END=875) (TABLE(I,J),J=31,40)
      READ (UNIT=4,FMT=997,END=875) (TABLE(I,J),J=41,50)
      READ (UNIT=4,FMT=997,END=875) (TABLE(I,J),J=51,60)
      READ (UNIT=4,FMT=993,END=875) (TABLE(I,J),J=61,63)
  997 FORMAT (10F8.2)
  993 FORMAT (3F8.2)
  998 CONTINUE
  875 DO 9 I=1,NN
      PRINT*,'-----------------------------------------------------'
      PRINT*,'THE UNIFAC METHOD NEEDS FUNCTIONAL GROUPS OF COMPOUNDS'
      PRINT*,'THE CHOICE OF POSSIBLE GROUPS IS ARBITRARY AND LIMITED'
      PRINT*,'WITH THE FOLLOWING GROUPS                             '
      PRINT*,(COMP(L),L=1,10)
      PRINT*,(COMP(L),L=10,20)
      PRINT*,(COMP(L),L=20,30)
      PRINT*,(COMP(L),L=30,40)
      PRINT*,(COMP(L),L=40,50)
      PRINT*,(COMP(L),L=50,60)
      PRINT*,(COMP(L),L=60,63)
      PRINT*,'----------------------------------------------------'
      J=1
      SUMC=0
  130 PRINT*,'ENTER THE NAME OF UNIFAC GROUPS IN COMPONENT ',NAME(I)
      READ (*,10) CM1
      PRINT*,CM1
   10 FORMAT (A6)
      IF (CM1.EQ.'END') GO TO 991
      IF (CM1.EQ.'NEW') GO TO 991
      IDX1=FINDR(CM1,COMP)
      IF (IDX1.EQ.-1) GO TO 130
      PRINT*,'ENTER THE NUMBER OF GROUPS OF THIS KIND'
      READ (*,11) KV
      PRINT*,KV
   11 FORMAT (I2)
      ITAB(I,J)=IDX1
      RB(I,J)=RQ(IDX1,1)
      QB(I,J)=RQ(IDX1,2)
      KQR(I,J)=KV
      MNR(I)=SUMC+KV
      SUMC=MNR(I)
      J=J+1
      GO TO 130
  991 KONT(I)=J-1
    9 CONTINUE
```

```
C       DO 775 I=1,NN
C       DO 775 M=1,KONT(I)
C       DO 775 J=1,NN
C       DO 775 N=1,KONT(J)
C       PRINT*,'TABLE(',I,M,J,N,')= ',TABLE(ITAB(I,M),ITAB(J,N))
C 775   CONTINUE
  910   RETURN
        END
C
        SUBROUTINE RFUGNC(T,TC,PC,FHN)
C
        TR=T/TC
        FHNOP=7.224-7.534/TR-2.548*ALOG(TR)
        FHN=PC*EXP(FHNOP)
        RETURN
        END
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```