Thermochimica Acta 490 (2009) 37–42

Contents lists available at ScienceDirect

Thermochimica Acta

journal homepage: www.elsevier.com/locate/tca

Low pressure vapor–liquid equilibrium in ethanol + congener mixtures using the Wong–Sandler mixing rule

Claudio A. Faúndez[a], José O. Valderrama[b,c,*]

[a] Universidad de Concepción, Fac. de Ciencias Físicas y Matemáticas, Casilla 160-C, Concepción, Chile
[b] University of La Serena, Faculty of Engineering, Department of Mechanical Engineering, Casilla 554, La Serena, Chile
[c] Centro de Información Tecnológica, Casilla 724, La Serena, Chile

ARTICLE INFO

Article history:
Received 10 November 2008
Received in revised form 4 February 2009
Accepted 9 February 2009
Available online 21 February 2009

Keywords:
Vapor–liquid equilibrium
Alcoholic mixtures
Equations of state
Wong–Sandler mixing rule

ABSTRACT

Phase equilibrium in binary ethanol mixtures found in alcoholic beverage production has been analyzed using a cubic equation of state (EoS) and suitable mixing and combining rules. The main objective of the study is the accurate modeling of the congener concentration in the vapor phase (substances different from ethanol), considered to be an important enological parameter in the alcohol industry. The Peng–Robinson (PR) equation of state has been used and the Wong–Sandler (WS) mixing rules, that include a model for the excess Gibbs free energy, have been incorporated into the equation of state constants. In the Wong–Sandler mixing rules the van Laar (VL) model for the excess Gibbs energy has been used. This combination of equations of state, mixing rules and combining rules are commonly applied to high pressure phase equilibrium and have not yet been treated in a systematic way to complex low pressure ethanol mixtures as done in this work. Nine binary ethanol + congener mixtures have been considered for analysis. Comparison with available literature data is done and the accuracy of the calculations is discussed, concluding that the model used is accurate enough for engineering applications.

1. Introduction

In many applications in the food industry, such as the design of distillation processes in alcoholic beverage production, the knowledge of the equilibrium conditions of the mixtures involved in the separation processes are of special importance. This is so, because the driving force that produces separation of components is the difference between the actual concentration and the concentration at thermodynamic equilibrium. In wine and must distillation the great amount of substances found in the mixture to be distilled and the very low concentration of many other components (different from ethanol and water), called congeners, make it difficult to correlate and predict the concentration of the distilled product, considered to be the most important variable in the produced spirit. Several of the congener compounds are essential part of the aroma of the distilled product and therefore their concentrations are important enological parameters [1,2]. These congener substances are usually present in concentrations of part per million, 10^{-6} to 10^{-4} mg/L [3–5], factor that imposes an additional difficulty for modeling these mixtures.

As known, the problem of phase equilibrium consists of the calculation of some variables of the set (T, P, x, y), if some of them are known. For a vapor–liquid mixture at equilibrium conditions, the temperature and the pressure are the same in both phases, and the remaining variables are defined by the material balance and the "*fundamental equation of phase equilibrium*". For engineering purposes, this fundamental equation is usually expressed in terms of the fugacity of each component in the different phases present in the process [6]. Usually the treatment of low pressure vapor–liquid equilibrium (VLE) data is done using activity coefficient models, although the use of equations of state has also been attempted [7]. Both approaches require binary parameters to be determined from experimental data [8], usually isothermal data. However, many vapor–liquid equilibrium data, are presented in the literature at isobaric conditions. Therefore, a detailed analysis of the pressure effects on parameter calculations and on the accuracy of the correlations is of special importance to use these thermodynamic models in modeling, simulation and design of distillation processes. Therefore, isothermal data at varying pressures are used in this study.

Binary mixtures containing water + congener and ethanol + congener have been studied in the literature at atmospheric pressure using several activity coefficient models [9–12]. However, with the proposals of modern mixing rules such as those involving the excess Gibbs free energy, the equation of state (EoS) method has become more popular. This paper considers the study of nine

---

Abbreviations: EoS, equation of state; PR, Peng–Robinson; PR/WS/VL, Peng–Robinson + Wong–Sandler + van Laar model; VL, van Laar; WS, Wong–Sandler mixing rule; %Δ, percent deviation.

[*] Corresponding author. Tel.: +56 51 204205; fax: +56 51 551158.
E-mail address: jvalderr@userena.cl (J.O. Valderrama).

0040-6031/$ – see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.tca.2009.02.007

Nomenclature

A_{ij}	parameter in the van Laar model
a_c, b	parameter in the PR EOS
a_m, b_m	interaction parameters in the mixing rules
g^E	excess Gibbs free energy
k_{ij}	binary interaction parameter
P	pressure
P_c	critical pressure
R	ideal gas constant
T	temperature
T_c	critical temperature
T_R	reduced temperature
V	volume
y_1	mole fraction of congener in the vapor phase (component 1)
y^{calc}	calculated mole fraction of a congener in the vapor phase
y^{exp}	experimental mole fraction of a congener in the vapor phase
x_i	experimental mole fraction of congener in the liquid phase (component i)

Greek letters

$\alpha(T)$	temperature function in the PR EoS
ω	acentric factor

Super/subscripts

cal	calculated
exp	experimental
i, j	components i and j

isothermal data of binary mixtures ethanol + congener from 0.039 to 6.20 bar and the correlation of such data using an equation of state.

The nine congeners are, acetic acid, ethyl acetate, furfural, methanol, 2-methyl-1-propanol, 1-pentanol, 1-propanol, methyl acetate and propyl acetate. The thermodynamic model considered in this work is the Peng–Robinson (PR) equation of state with the mixing rules of Wong and Sandler (WS) [13], including the van Laar (VL) model for the Gibbs free energy included in the mixing rules. This model and all the equations that describe it are presented in the following section.

2. The thermodynamic model

One of the most commonly used methods for phase equilibrium correlation and prediction in complex systems is the application of an equation of state and appropriate mixing and combining rules to describe the concentration dependency of the parameters of the EoS. Of the many equations of state nowadays available, the so called cubic equations derived from van der Waals proposal such as the Peng–Robinson EoS [14], are widely used to treat these systems. The model proposed by Peng and Robinson can be written in a general form as follows:

$$P = \frac{RT}{V-b} - \frac{a_c\alpha(T_R)}{V(V+b)+b(V-b)} \tag{1}$$

In this equation, a_c and b are parameters, specific for each substance, determined using the critical properties, T_c and P_c. Also, $\alpha(T_R)$ is a function of the reduced temperature $T_R = T/T_c$ and of the acentric factor ω, as follows:

$$\begin{aligned} a_c &= 0.457235\left(\frac{R^2T_c^2}{P_c}\right) \\ b &= 0.077796\left(\frac{RT_c}{P_c}\right) \\ \alpha(T_R) &= [1+F(1-T_R^{0.5})]^2 \\ F &= 0.36646 + 1.54226\omega - 0.26992\omega^2 \end{aligned} \tag{2}$$

During the last three decades, efforts have been done on extending the applicability of cubic equations of state to obtain accurate representation of phase equilibria in many industrially important mixtures. The different approaches presented in the literature, include the use of multiple interaction parameters in the mixing rules, the introduction of the local-composition concept, and the use of non-quadratic mixing rules. More details on these different approaches are described elsewhere by the authors [7].

Another attractive way, which has been proposed to develop more accurate mixing rules, has been the combination of an EoS with a model for the excess Gibbs free energy (or activity coefficient model). Two main approaches have been used for applying these models. In the first approach, the link between the EoS and the excess Gibbs free energy model is done at infinite pressure [15,16]. In the second approach, the link between the EoS and the excess Gibbs free energy model is done at low or zero pressure [17].

In this work, the Peng–Robinson equation of state with the Wong–Sandler mixing rules has been used to correlate low pressure VLE data for ethanol + congener mixtures. The WS mixing rules for the Peng–Robinson EoS can be summarized as follows [13]:

$$\begin{aligned} b_m &= \frac{\displaystyle\sum_i^N\sum_j^N x_ix_j(b-(a/RT))_{ij}}{1-\displaystyle\sum_i^N x_ia_i/b_iRT - A_\infty^E(x)/\Omega RT} \\ \left(b-\frac{a}{RT}\right)_{ij} &= \frac{1}{2}[b_i+b_j] - \frac{\sqrt{a_ia_j}}{RT}(1-k_{ij}) \\ a_m &= b_m\left(\sum_i^N\frac{x_ia_i}{b_i} + \frac{A_\infty^E(x)}{\Omega}\right) \end{aligned} \tag{3}$$

In these equations, k_{ij} is an interaction parameter, $\Omega = 0.34657$ for the Peng–Robinson EoS, and $A_\infty^E(y)$ is calculated assuming that $A_\infty^E(y) \approx A_0^E(y) \approx g^E$. For g^E several models have been used in the literature. In this work g^E has been calculated using the van Laar model.

The van Laar model, detailed in Table 1 contains two empirical parameters for a binary mixture. Therefore, for a binary mixture the WS mixing rule includes one adjustable binary interaction parameter k_{12} for $(b-a/RT)_{ij}$, besides the two parameters, A_{12} and A_{21}, included in the g^E model. These three adjustable parameters for

Table 1
van Laar model for the Gibbs free energy used in the Wong–Sandler mixing rule.

van Laar model
$\frac{g^E}{RT} = \sum_i^N y_i \frac{\sum_j^N y_jA_{ij}}{1-x_i}\left[1 - \frac{y_i\sum_j^N y_jA_{ij}}{y_i\sum_j^N y_jA_{ij} + (1-y_i)x_i\sum_j^N y_jA_{ji}}\right]^2$
For a binary mixture:
$\frac{g_0^E}{RT} = \frac{(A_{12}/RT)y_1y_2}{y_1(A_{12}/A_{21})+y_2}$

each of the mixtures have been determined using experimental phase equilibrium data at constant temperature, available in the literature. In summary, the thermodynamic model includes the Peng–Robinson equation of state, the Wong–Sandler mixing rule, and the van Laar model for g^E in the mixing rules, model designated as PR/WS/VL in the rest of the paper.

The Peng–Robinson EoS with the Wong–Sandler mixing rules have been used in several applications, mainly vapor–liquid equilibria at high pressure and liquid–liquid equilibrium at low and high pressure [7,13]. To the best of the author's knowledge there is no application of this combined PR/WS/VL model to correlate low-pressure vapor-equilibrium data of ethanol mixtures. Therefore the analysis done in this study represents a new application of modern mixing rules combined with equations of state to treat low pressure alcoholic mixtures for simulation and design purposes.

3. Mixtures studied

Nine binary ethanol + congener mixtures were considered for the study. The congeners included in these mixtures are acetic acid, ethyl acetate, furfural, methanol, 2-methyl-1-propanol, 1-pentanol, 1-propanol, methyl acetate and propyl acetate. Table 2 shows pure component properties for all the substances involved in this study. In the Table, M is the molecular weight, T_b is the normal boiling temperature, T_c is the critical temperature, P_c is the critical pressure, V_c is the critical volume and ω is the acentric factor. The values for these properties, were obtained from [18].

Table 3 gives some details on the experimental data used in the study including the literature source for each data set [19,20]. In this Table, T is the temperature (expressed in Kelvin), N is the number of experimental data, P is the pressure (expressed in bar), Δx_1 is the liquid mole fraction range for component 1 and Δy_1 is the vapor mole fraction range for component 1. As seen in Table 3, data for 28 isotherms with a total of 301 data points were considered. The temperature ranges from 298 to 393 K and the pressure from 0.039 to 6.20 bar.

Bubble pressure calculations for binary mixtures were performed using the PR/WS/VL model. The adjustable parameters (k_{12}, A_{12}, A_{21}) of the model were determined by optimization of the objective function given by Eqn. (4). The program designed considers the use of the Levenberg–Marquardt algorithm [21] as the optimization method. The objective function was defined as the relative error between calculated and experimental values of the pressure:

$$F = \sum_{i=1}^{N} \left| \frac{P_i^{\mathrm{cal}} - P_i^{\mathrm{exp}}}{P_i^{\mathrm{exp}}} \right| \tag{4}$$

In this equation N is the number of points in the experimental data set and P is the bubble pressure.

4. Results and discussion

Table 4 shows the optimum binary interaction parameters in the Wong–Sandler mixing rules at all temperatures studied. The Table 5 shows the results for the pressure and the vapor mole fraction of congeners for the nine binary mixtures studied using the PR/WS/VL model. In this table, the average absolute deviations for the pressure, $|\%\Delta P|$, and the average and relative deviations for the congener concentration in the vapor phase, $|\%\Delta y_1|$ and $\%\Delta y_1$ for the PR/WS/VL model are given.

The average deviations $|\%\Delta P|$, $|\%\Delta y_1|$, and relative deviations $\%\Delta y_1$, for a set of N data, given in the tables, are defined as:

$$|\%\Delta P| = \frac{100}{N} \sum \left| \frac{P^{\mathrm{cal}} - P^{\mathrm{exp}}}{P^{\mathrm{exp}}} \right|_i \tag{5}$$

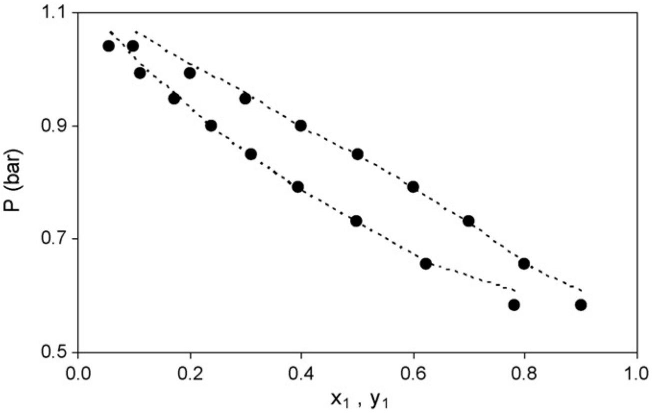

Fig. 1. Experimental (●) and calculated values (—) of bubble pressure P vs liquid mole fraction x_1 and vapor mole fraction y_1 for the system 1-propanol (1) + ethanol (2) at $T = 353$ K.

$$|\%\Delta y_1| = \frac{100}{N} \sum \left| \frac{y_1^{\mathrm{cal}} - y_1^{\mathrm{exp}}}{y_1^{\mathrm{exp}}} \right|_i \tag{6}$$

$$\%\Delta y_1 = \frac{100}{N} \sum \left| \frac{y_1^{\mathrm{cal}} - y_1^{\mathrm{exp}}}{y_1^{\mathrm{exp}}} \right|_i \tag{7}$$

As seen in Table 5, the PR/WS/VL model reproduces the bubble pressures of these binary mixtures with mean absolute deviations less than 12.1% for any temperature. The calculated pressure was calculated with deviations between 0.7% and 12.0%. In 22 isotherms, pressure deviations are below 4.1%, and in another three isotherms deviation are below 8.0%.

With respect to the congener concentration in the vapor phase y_1, this quantity is predicted in all cases studied, with mean absolute deviations from 0.8% to 12.9%. In most cases studied, the absolute average deviations of y_1 are less than 10.3%. Relative deviations vary between −11.5% and 12.1% and for only two cases deviations are higher than 10%. The maximum individual deviation in y_1 is 28.4%, for a single point for the system furfural (1) + ethanol (2) at 323 K. It should be mentioned that the highest deviations are generally found for those cases in which the congener concentration in the vapor phase is very low.

Figs. 1 and 2 shows the bubble pressure vs concentration for the mixture 1-propanol (1) + ethanol (2) at $T = 353$ K, and for 2-methyl-1-propanol (1) + ethanol (2) at $T = 323$ K, respectively. The symbol (●) represents the experimental data and the dashed line (- - -) represents the calculated values. It can be seen that there is

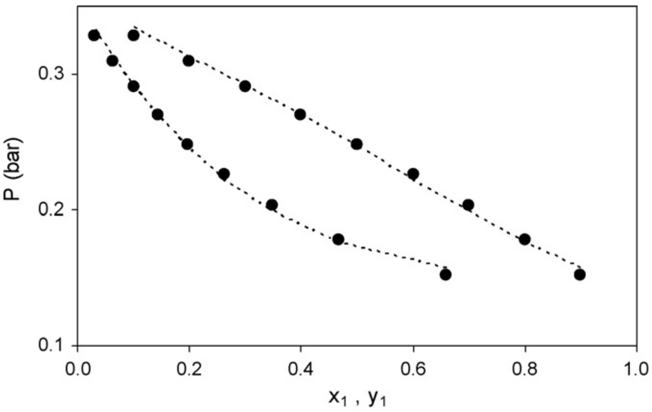

Fig. 2. Experimental (●) and calculated values (—) of bubble pressure P vs liquid mole fraction x_1 and vapor mole fraction y_1 for the system 2-methyl-1-propanol (1) + ethanol (2) at $T = 323$ K.

Table 2
Properties for all substances involved in this study.

Components	M (kg/kg mol)	T_b (K)	T_c (K)	P_c (bar)	V_c (m^3/kmol)	ω
Ethanol	46.1	351.45	513.95	61.37	0.168	0.6436
Acetic acid	60.1	391.05	591.95	57.86	0.180	0.4665
Ethyl acetate	88.1	350.25	523.35	38.80	0.286	0.3664
Furfural	96.1	434.85	670.15	56.60	0.252	0.3678
Methanol	32.0	337.85	512.65	80.84	0.117	0.5659
2-Methyl-1-propanol	74.1	380.85	547.75	49.95	0.274	0.5857
1-Pentanol	88.2	410.95	588.10	38.97	0.326	0.5731
1-Propanol	60.1	370.35	536.75	51.69	0.218	0.6204
Methyl acetate	74.1	330.09	506.55	47.50	0.228	0.3313
Propyl acetate	102.1	374.65	549.73	33.60	0.345	0.3839

Table 3
Details on the phase equilibrium data for the systems considered in this study. In the table the temperature values have been rounded to the closest integer. For the mixture propyl acetate + ethanol, vapor mole fraction was not available.

Systems ethanol (2) +	Ref.	T (K)	N	Range of date		
				P (bar)	Δx_1	Δy_1
Acetic acid	[19]	308	13	0.0387–0.1062	0.2380–0.9400	0.0350–0.8860
		318	12	0.0633–0.1765	0.2380–0.9320	0.0380–0.8710
Ethyl acetate	[19]	313	14	0.1820–0.2842	0.0060–0.9600	0.0220–0.9280
		328	14	0.3789–0.5358	0.0055–0.9440	0.0185–0.9020
		333	19	0.4812–0.6465	0.0505–0.9760	0.1100–0.9393
		343	15	0.7312–0.9493	0.0065–0.9750	0.0175–0.9480
Furfural	[19]	323	9	0.0387–0.2932	0.0201–0.9800	0.0046–0.3240
		338	9	0.0746–0.5598	0.0201–0.9800	0.0048–0.3510
		353	9	0.1333–1.0730	0.0201–0.9800	0.0051–0.3603
Methanol	[19]	298	11	0.0856–0.1612	0.0841–0.9165	0.1610–0.9610
		373	10	2.3293–3.4465	0.0620–0.9410	0.0890–0.9610
		393	10	4.2774–6.2037	0.0610–0.9420	0.0820–0.9590
2-Methyl-1-propanol	[19]	323	9	0.1022–0.2783	0.1000–0.9000	0.0310–0.6600
		333	9	0.1711–0.4436	0.1000–0.9000	0.0330–0.6750
		343	9	0.2751–0.6879	0.1000–0.9000	0.0350–0.6870
		353	9	0.4291–1.0253	0.1000–0.9000	0.0370–0.7010
1-Pentanol	[20]	348	19	0.1352–0.8489	0.0500–0.9500	0.0070–0.6610
1-Propanol	[19]	323	9	0.1440–0.2823	0.1000–0.9000	0.0480–0.7580
		333	9	0.2374–0.4508	0.1000–0.9000	0.0510–0.7680
		343	9	0.3819–0.7011	0.1000–0.9000	0.0530–0.7770
		353	9	0.5825–1.0398	0.1000–0.9000	0.0550–0.7820
Methyl acetate	[19]	323	8	0.3212–0.7598	0.0269–0.9217	0.1101–0.9511
		333	8	0.4932–1.0796	0.0269–0.9217	0.1066–0.9480
		343	8	0.7731–1.5088	0.0269–0.9217	0.1052–0.9449
		353	8	1.1463–2.0660	0.0269–0.9217	0.0842–0.9430
Propyl acetate	[19]	323	11	0.1790–0.3139	0.0500–0.9500	*
		333	11	0.2729–0.4869	0.0500–0.9500	*
		343	11	0.4089–0.7358	0.0500–0.9500	*

good agreement between model estimates and experimental data, as described above.

Fig. 3 shows the individual relative deviations of the predicted congener concentration in the vapor phase (y_1) in the mixture ethyl acetate (1) + ethanol (2) at 328 K (●) and 343 K (△). Experimental data are from the Dechema Data Base [19] and the calculated values are with the PR/WS/VL model. It can be observed that there is good agreement between correlated and experimental values. The individual deviations found for y_1 are less than 9.0% for most points, with a few exceptions at lowest experimental congener concentration.

There are some cases, however, in which deviations seem to be unacceptable higher, such as the cases acetic acid (1) + ethanol (2) and 2-mehtyl-1-propanol (1) + ethanol (2). For the same cases using different models very variable results have been published in the literature, both for the variables being correlated and for the parameters of the models used. These facts give and indication about the complexity of the systems being correlated. The DECHEMA collection for instance [19], from where the data treated in this work

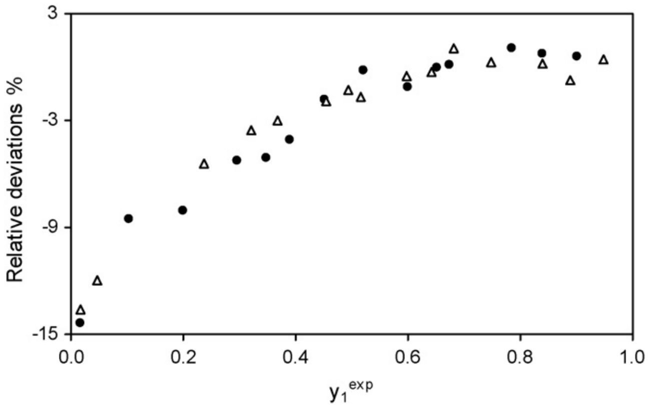

Fig. 3. Individual relative deviations of the predicted congener concentration in the vapor phase (y_1) in the mixture ethyl acetate (1) + ethanol (2) at 328 K (●) and 343 K (△).

Table 4
Optimum binary interaction parameter and van Laar constants in the Wong–Sandler mixing rules at all temperatures studied.

Systems ethanol (2) +	T (K)	A_{12}	A_{21}	k_{12}
Acetic acid	308	−0.9983	−0.9979	0.0058
	318	−0.9902	−0.9937	−0.0563
Ethyl acetate	313	0.9980	1.0000	0.0933
	328	0.9389	0.9568	0.0848
	333	2.3435	0.0706	0.2192
	343	0.7526	0.8988	0.1089
Furfural	323	0.9635	0.9922	0.2906
	338	0.1935	1.0935	0.4420
	353	0.2220	1.0328	0.4454
Methanol	298	0.0266	1.1000	0.0977
	373	0.1203	0.1124	−0.0552
	393	1.4996	1.7251	−0.5881
2-Methyl-1-propanol	323	−1.1044	−1.0180	0.3187
	333	−0.9412	−0.9660	0.2806
	343	−0.6302	−0.8438	0.2323
	353	−0.9685	−0.9046	0.3175
1-Pentanol	348	0.2560	0.1797	0.0446
1-Propanol	323	0.2156	0.1462	−0.0979
	333	−0.0421	1.1015	0.0205
	343	−0.0434	1.1001	0.0483
	353	−0.0397	1.0984	0.0587
Methyl acetate	323	0.2070	0.2590	0.1406
	333	0.2202	0.2592	0.1732
	343	1.1455	1.2298	−0.0901
	353	0.1374	1.0453	0.2139
Propyl acetate	323	0.9445	0.9687	0.1520
	333	0.9115	1.0309	0.1111
	343	0.8979	1.0638	0.1059

Table 5
Average deviations for the pressure and vapor mole fraction of component (1) using the PR/WS/VL model.

Systems ethanol (2) +	T (K)	% ΔP	$\lvert\%\Delta y_1\rvert$	$\%\Delta y_1$
Acetic acid	308	11.9	12.9	−11.5
	318	11.0	8.9	−8.9
Ethyl acetate	313	0.9	1.9	−1.3
	328	0.9	3.6	−3.3
	333	7.4	10.2	−10.0
	343	0.7	3.1	−2.8
Furfural	323	12.0	12.5	−9.5
	338	7.0	9.5	−8.9
	353	6.6	6.1	−2.8
Methanol	298	3.4	2.6	−0.2
	373	1.3	1.1	−0.9
	393	1.7	0.8	−0.2
2-Methyl-1-propanol	323	1.8	12.1	12.1
	333	2.1	8.3	8.2
	343	1.7	6.6	6.6
	353	1.5	4.6	4.5
1-Pentanol	348	1.8	7.6	6.8
1-Propanol	323	2.1	8.3	7.1
	333	1.6	4.3	3.2
	343	1.2	3.0	2.1
	353	1.4	2.5	1.9
Methyl acetate	323	1.1	2.3	−2.3
	333	3.3	2.5	−1.3
	343	2.1	2.5	−1.9
	353	4.0	1.7	−1.7
Propyl acetate	323	1.0	- - -	- - -
	333	1.5	- - -	- - -
	343	1.2	- - -	- - -

were obtained, gives deviations for the vapor phase concentration much higher than the values found using the PR/WS/VL model, for some mixtures, while for others similar and lower deviations are found. For the mixtures mentioned above similarly high deviations are found, For others, such as furfural (1) + ethanol (2) at 323 K the DECHEMA collection gives a deviation of 18.9% (this work is 12.5%), and for the mixture 1-propanol (1) + ethanol (2) at 353 K the collection gives 1.1% (this work 2.5%). The values taken from the DECHEMA collection are for the van Laar model.

The authors [10] analyzed similar systems using the Gamma–Phi method using two activity coefficient models (NRTL and UNIFAC) and one model similar to the one used here, the PSRK equation. Results, in the average, are lower with the model proposed here, in particular when comparing the PSRK with the PR/WS/VL model used in this work.

5. Conclusions

Vapor–liquid equilibrium in mixtures ethanol + congener has been modeled using the equation of state method (Peng–Robinson + Wong–Sandler + van Laar). The study and the results allow obtaining three main conclusions: (i) the equation of state method using appropriate mixing rules such as the one of Wong and Sandler can be used to model low pressure complex mixtures; (ii) bubble pressures can be obtained with good accuracy with the PR/WS/VL model, giving absolute average deviations below 12.1% for each isothermal data set and the overall absolute average deviations is 3.4%; (iii) the congener concentration in the vapor phase, y_1, can be obtained with good accuracy, giving absolute average deviations bellow 13.0% for each isothermal data set and the overall absolute average deviations and relative average deviations are 5.8% and 0.4%, respectively.

Acknowledgments

The authors thank the National Council for Scientific and Technological Research, CONICYT, for its grant FONDECYT 3020020 and the Center for Technological Information (La Serena-Chile) for computer and library support. CAF thanks the Department of Physics of the University of Concepción for special support during the development of this work. JOV thanks the Direction of Research of the University of La Serena for permanent support.

References

[1] A. Hikari, R. Kubo, J. Chem. Eng. Jpn. 8 (1975) 294–299.
[2] M.P.Y. Lillo, E. Latrille, G. Casaubon, E. Agosin, E. Bordeu, N. Martin, Food Qual. Preference 16 (January) (2005) 59–70.
[3] J. Lora, M.I. Iborra, R. Perez, I. Carbonell, Rev. Esp. Cien. Tec. Ali. 32 (1992) 621–633.
[4] C.A. Faúndez, V.H. Alvarez, J.O. Valderrama, Thermochim. Acta 450 (2006) 110–117.
[5] V. Athès, P. Paricaud, M. Ellaite, J. Souchon, W. Fürst, Fluid Phase Equilib. 265 (2008) 139–154.
[6] J.M. Prausnitz, R.N. Lichtenthaler, E. Gomes de Azevedo, Molecular Thermodynamics of Fluid-Phase Equilibria, Prentice Hall International Series, New Jersey, USA, 1999.
[7] J.O. Valderrama, Ind. Eng. Chem. Res. 42 (2003) 1603–1618.
[8] S.M. Walas, Phase Equilibria in Chemical Engineering, Butterworth Pub., Storeham, USA, 1985.
[9] J.O. Valderrama, C. Pizarro, R. Rojas, Alimentaria 39 (2001) 151–156.
[10] C.A. Faúndez, J.O. Valderrama, J. Food Eng. 65 (2004) 577–583.
[11] C.A. Faúndez, V.H. Alvarez, J.O. Valderrama, J. Phase Equilib. Diff. 25 (2004) 230–236.
[12] V.H. Alvarez, C.A. Faúndez, J.O. Valderrama, Can. J. Chem. Eng. 83 (2005) 485–492.
[13] H. Orbey, S.I. Sandler, Modeling Vapor–Liquid Equilibria. Cubic Equations of State and Their Mixing Rules, Cambridge University Press, USA, 1998.
[14] D.Y. Peng, D.B. Robinson, Ind. Eng. Chem. Fundam. 15 (1976) 59–64.
[15] M.I. Huron, J. Vidal, Fluid Phase Equilib. 3 (1979) 255–271.
[16] D.S. Wong, S.I. Sandler, AIChE J. 38 (1992) 671–680.
[17] S. Dahl, M.L. Michelsen, AIChE J. 36 (1990) 1829–1836.
[18] T.E. Daubert, R.P. Danner, H.M. Sibul, C.C. Stebbins, Physical and Thermodynamic Properties of pure Chemicals. Data Compilation, Taylor & Francis, London, UK, 1996.
[19] J. Gmehling, U. Onken, W. Arlt, Vapor–liquid Equilibrium Data Collection, DECHEMA, Frankfurt, Germany, 1982.
[20] S. Ohe, Vapor–Liquid Equilibrium Data, Physical Sciences Data 37, Kodansha Ltd., Elsevier Science Publishers B.V., Tokyo, Amsterdam, 1989.
[21] M. Reilly, Computer Programs for Chemical Engineering Education, vol. 2, Sterling Swift, TX, USA, 1972.