

High-temperature vapour–liquid equilibrium for ethanol–1-propanol mixtures and modeling with SAFT-VR



A.F. Cristino^a, P. Morgado^b, A. Galindo^c, E.J.M. Filipe^b, A.M.F. Palavra^b,
C.A. Nieto de Castro^{a,*}

^a Centro de Química Estrutural, Faculdade de Ciências, Universidade de Lisboa, Campo Grande, 1749-016 Lisboa, Portugal

^b Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, 1049-001 Lisboa, Portugal

^c Department of Chemical Engineering and Centre for Process System Engineering, Imperial College London, South Kensington Campus, London SW7 2AZ, UK

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ABSTRACT

Alcohols have a wide use in industry, and some of them are solvents for fats, oils, resins, paints, and nitrocellulose; on the other hand, others find use in the manufacture of perfumes and brake fluids. Mixtures of ethanol with 1-propanol, 1-butanol, or 1-pentanol can be used as fuel oxygenates. In addition these mixtures can be used as cryogenic fluids and as heat reservoir in cryogenic power generation systems. This justifies the importance of the knowledge of thermodynamic properties for these mixtures at various temperatures. However, properties like experimental densities, and vapour liquid equilibrium at high temperatures, for some alcohols mixtures are scarce, and when they exist do not have the claimed accuracy.

This paper reports VLE measurements for the system ethanol + 1-propanol at temperatures and pressures up to 423 K and 1 MPa, respectively, performed at our laboratories. The statistical associating fluid theory for potentials of variable range (SAFT-VR) was used to model the systems and found to accurately reproduce the experimental data.

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1. Introduction

Many engineering problems require the knowledge of several thermodynamic and transport properties, such as heat and mass transfer coefficients, density, heat capacity, viscosity and thermal conductivity. However, the laboratory work behind such measurements is laborious and time consuming. Despite this limitation, these measurements are necessary not only for the design of chemical engineering processes [1–3], but also to check new theories about the liquid state.

In the last three decades or more, experimental programmes to measure vapour–liquid equilibria (VLE) were developed all over the world. There were numerous apparatus built to fill this need. This has provided the scientific community with a lot of experimental studies at low and room temperatures [4,5]. However for higher temperatures, the situation is rather different, because the data are scarce, and often of lower accuracy. Nowadays it is possible to acquire more accurate experimental data, by using more

convenient experimental techniques and more accurate measurements of pressure, temperature and composition.

A VLE experimental program at high temperatures was developed in collaboration between the Centre for Molecular Sciences and Materials (CCMM-FCUL) and the Experimental Thermodynamics Laboratory (CQE-IST). We have studied systems like water + ethanol [6] and water + 1-propanol [7]. The production of biodegradable fuels needs accurate measurements on water + alcohol systems, such as methanol, ethanol, propanol, butanol (linear and branched) at high temperatures. On the other hand, biodegradable fuels start to play an important role in the world global economy, as oil prices are increasing steadily and the search for alternative energies and new fuels is vital for the sustainability of the world economy.

In this work we completed the cycle of binary mixtures with water, ethanol and 1-propanol, by studying the binary mixture ethanol + 1-propanol. To the best of our knowledge, there is no reliable data for this system at high temperatures. The vapour pressures of ethanol and 1-propanol were analyzed using the Wagner equation [8].

As in previous work, we have used the statistical associating fluid theory for potentials of variable range (SAFT-VR) equation to model the experimental results. SAFT is a molecular-based

* Corresponding author. Tel.: +351 217 500 918; fax: +351 217 500 088.
E-mail address: cacastro@ciencias.ulisboa.pt (C.A. Nieto de Castro).

Table 1
Provenance, purity and water content of the materials.

	Supplier	Mass fraction purity	Purification	Water content measured by supplier
Ethanol	Panreac	>0.999	None	<1000 ppm
1-Propanol	Fisher Scientific	>0.999	Dried with anhydrous copper sulphate	<1000 ppm
Tetrachloroethylene	H&D Fitzgerald	>0.990	Density certified ampoules	Not specified

equation of state (EOS), which explicitly takes into account the contribution of molecular structure, i.e. shape, association and polarity [9–11]. Within the SAFT framework, the free energy of the system is written as the sum of separate contributions:

$$A = A^{\text{ideal}} + A^{\text{mono}} + A^{\text{chain}} + A^{\text{assoc}} \quad (1)$$

where A^{ideal} is the ideal free energy, A^{mono} the contribution to the free energy due to the monomer segments, A^{chain} the contribution due to the formation of bonds between monomer segments and A^{assoc} the contribution due to association interactions. The different versions of SAFT essentially correspond to different choices for the monomer fluid and different theoretical approaches to calculate the monomer free energy and structure. In this work, we have used, SAFT-VR, in which molecules are described as homonuclear chains of spherical monomers interacting through a potential of variable range, in this case a square well [12,13].

The SAFT-VR equation has been successfully used to describe the phase equilibria of a wide range of industrially important systems, from alkanes of low molecular weight to simple polymers, perfluoroalkanes, refrigerants, carbon dioxide, water, electrolyte solutions, etc. (see Ref. [14] and references therein).

Systems involving alcohols have been successfully modeled with SAFT-VR, especially focusing on the phase behaviour of (water + alcohol) mixtures. Patel [15] studied the phase equilibria of (water + alcohol) binary mixtures and of ternary (water + alcohol + salt mixtures), including in the theory the description of electrolytes. Mac Dowell et al. [16] modeled the (water + ethanol) mixture as a starting point for developing an accurate theoretical model of ethanolamine. Very recently, Schreckenberget al. [17] published a study on the thermodynamic and solvation properties of electrolyte solutions with SAFT-VR, including (water + alcohol) mixed solvents. In these studies, hydrogen bonding of alcohols was accounted by three association sites in each alcohol molecule, one representing the hydroxyl hydrogen atom and the other two, the oxygen unbound electron pairs; this scheme, in which association is only permitted between unlike sites, is usually referred as 3B.

Regarding mixtures of alcohols, de Villiers et al. [18] used a different version of SAFT (sPC-SAFT) to study the behaviour of mixtures of alcohols with alkanes, water and other alcohols. They proposed a new association scheme for the alcohols, which improves the description of water + alcohol mixtures without compromising the performance of the EOS for the other systems. The same group has very recently extended this line of work, explicitly including the effect of polarity in the theory [19]. In this work the (ethanol + 1-propanol) mixture was treated using the model presented by Mac Dowell et al. [16] for ethanol and for 1-propanol that developed by Patel [15].

2. Experimental

VLE measurements were carried out in the temperature range 363 K to 443 K and pressures up to 1 MPa, using a flow apparatus [6] which is an improved version of that described in a previous paper [20]. The main modifications were related with the pressure measurements and their uncertainty. The equilibrium pressure is now read using two pressure transducers (GE Druck, Model UNIK5000) with ranges of 0–0.4 and 0–1.7 MPa with uncertainties of 0.0002 MPa and 0.0009 MPa respectively, with two digital

pressure readouts ($4^{1/2}$ digits, GE Druck Model DPI282). The temperature was measured with a platinum resistance thermometer with an uncertainty of 0.1 K.

The VLE apparatus uses a flow method to minimize the thermal degradation of the samples, and is divided in three main sections. The first one involves the process of sample feeding in the system, the second one consists on the isothermal bath, where the equilibrium cell is maintained at the desired temperature. Finally, section three incorporates the vapour and liquid phase sampling, for composition determination. The mixture to be studied is introduced in a glass vessel and a sample is pumped to the preheater using a metering pump and to a second heat exchanger used for a fine tuning of the temperature of the sample before entering the windowed equilibrium cell which is inside the oven. The window permits the visualization of the vapour–liquid interface. The input line to the cell is made in an inverted U shape to increase the heat and mass transfer between the two phases after the liquid flash. The thermostat is an air bath controlled by a PID controller.

When the steady state is reached, the pressure and the temperature are measured and the liquid and vapour samples are collected. The vapour phase is removed from the top of the cell, using a micro-metering valve to expand it to atmospheric pressure. This metering valve also determines the vapour flow rate. The vapour after cooled and condensed in the heat exchanger is collected in a glass flask at atmospheric pressure and ice temperatures, to avoid evaporation, prepared for the density determination. The liquid sample is obtained from the bottom of the equilibrium cell and after passing through a condenser is expanded to the atmospheric pressure using also a micro-metering valve, and then collected also in an iced glass vessel for the density determination.

The provenance, purity and water content of the materials used in this work are presented in Table 1. Ethanol and 1-propanol had a confirmed purity greater than 99.9 wt% Tetrachloroethylene was supplied by H&D Fitzgerald as a certified reference material for liquid density (<https://density.co.uk/products/liquid-standards/>) with confirmed purity greater than 99 wt% [6]. The water content of the alcohol samples was measured by Coulometric Karl–Fisher analysis (Metrohm 831 KF Coulometer) and estimated to be smaller than 300 ppm (0.03%), a value that falls within the uncertainty of the molar fraction determination.

Liquid and vapour phase composition were determined indirectly by densimetry, calibrated according to the methodology described by Lampreia and Nieto de Castro [21]. Densities of the collected vapour and liquid samples were measured with an Anton Paar DSA 5000 M densimeter at atmospheric pressure and 293.15 K. The densimeter was calibrated with water (Deionised and degassed before use – Lab Production (Milli-Q), with a resistivity of $180 \text{ k}\Omega \times \text{m}$) and tetrachloroethylene with an expanded uncertainty of 0.01 kg m^{-3} ($k=2$)¹, at atmospheric pressure, between 283.15 and 323.15 K. Furthermore, the calibration curve as a function of composition (third order polynomial of the molar function of ethanol) was obtained from published data

¹ The expanded uncertainty, U was assumed for an infinite number of degrees of freedom, $k=2$, i.e. $U=2u$, where u is the uncertainty of the measurement.

Table 2SAFT-VR model parameters used in this work. The energy parameters are divided by Boltzmann's constant k_B .

	m	σ (Å)	ε/k_B (K)	λ	H-sites	e-sites	$\varepsilon_{ab}^{HB}/k_B$ (K)	K_{ab}^{HB} (Å ³)
Ethanol [18]	1.533	3.7150	244.417	1.6730	1	2	2357.79	0.14564
1-propanol [19]	1.8667	3.7571	215.012	1.7019	1	2	2499.96	0.19621

[22]. Using this analytical method the uncertainty of the molar fraction determination is 0.0001.

3. Theory

A quantitative interpretation of the results was performed using the molecular-based statistical associating fluid theory for potentials of variable attractive range, SAFT-VR. Only a very brief description of the model will be given here and the full expressions for the SAFT-VR equation of state can be found in the original references [12,13].

In the SAFT-VR approach, molecules are modelled as chains of m tangentially bonded hard spherical segments, with the attractive dispersive interactions described by a potential of variable attractive range such as the square-well potential used in this work. Each segment is characterized by three parameters, namely, the hard-sphere diameter σ and the depth ε and width λ of the potential well. In the case of associating molecules, such as ethanol and 1-propanol, which are hydrogen-bonding, embedded attractive square-well sites are included in the model, defined by their bonding volume K_{ab}^{HB} and the depth of the attractive potential ε_{ab}^{HB} .

As usual, the molecular model parameters for the pure substances are determined by minimization of the differences between theoretical and experimental properties, normally the liquid density and vapour pressure over the whole liquid–vapour range. The model used here for ethanol was presented by Mac Dowell et al. [16] and for 1-propanol we have used the model developed by Patel [15]. The full set of model parameters used for the studied substances are presented in Table 2.

For both alcohols, one association site representing the hydroxyl hydrogen atom and two representing the oxygen lone electron pairs are included. It should be noted that, both in the pure compounds and in the mixture, the associative interactions are only allowed between sites of different type, namely “hydrogen-type” sites can only interact with “electron-type” sites and vice-versa.

For the interactions between segments of different molecules, the unlike interaction ranges and volumes are determined by the

arithmetic average of the pure component parameters and the unlike interaction energies by the geometric average:

$$\sigma_{ij} = \frac{\sigma_{ii} + \sigma_{jj}}{2} \quad (2)$$

$$\lambda_{ij} = \frac{\lambda_{ii}\sigma_{ii} + \lambda_{jj}\sigma_{jj}}{\sigma_{ii} + \sigma_{jj}} \quad (3)$$

$$K_{ab,ij} = \left[\frac{K_{ab,ii}^{1/3} + K_{ab,jj}^{1/3}}{2} \right]^3 \quad (4)$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_{ii}\varepsilon_{jj}} \quad (5)$$

$$\varepsilon_{ab,ij}^{HB} = \sqrt{\varepsilon_{ab,ii}^{HB}\varepsilon_{ab,jj}^{HB}} \quad (6)$$

In this work, it was found that quantitative agreement between the theoretical and experimental results were obtained without the use of any correction factors to the above combination rules. This result reflects the similarity between the two studied substances and makes the theoretical description of the studied system fully predictive.

4. Results and discussion

In Table 3 our experimental measurements for mixtures of ethanol and 1-propanol of different composition at the temperatures 403.2, 413.2 and 423.2 K are presented. The theoretical predictions from the SAFT-VR EOS are presented in Fig. 1 along with the experimental data from this work. As can be seen, the overall agreement between the theoretical predictions and the experimental results, is very good, although the vapour pressure of

Table 3Vapour pressure of the ethanol (1)+1-propanol (2) system at 403.2, 413.2 and 423.2 K.^a

p (MPa)	x_1	y_1	p (MPa)	x_1	y_1
$T = 403.2$ K					
0.3042	0.0011	0.0019	0.4166	0.4290	0.5744
0.3198	0.0426	0.0754	0.4874	0.6919	0.7974
0.3846	0.2914	0.4042	0.5576	0.9983	0.9993
$T = 413.2$ K					
0.4080	0.0007	0.0022	0.5641	0.4563	0.5959
0.4290	0.0513	0.0747	0.6404	0.7001	0.8014
0.4939	0.2541	0.3642	0.7363	0.9998	0.9995
$T = 423.2$ K					
0.5461	0.0007	0.0026	0.7253	0.4553	0.5846
0.5653	0.0496	0.0714	0.8220	0.6916	0.7879
0.6483	0.2617	0.3608	0.9674	0.9983	0.9993

^a $u(T) = 0.1$ K, $u(p < 0.4) = 0.0002$ MPa, $u(p > 0.4) = 0.0009$ MPa, and $u(x_1) = u(y_1) = 0.0001$.

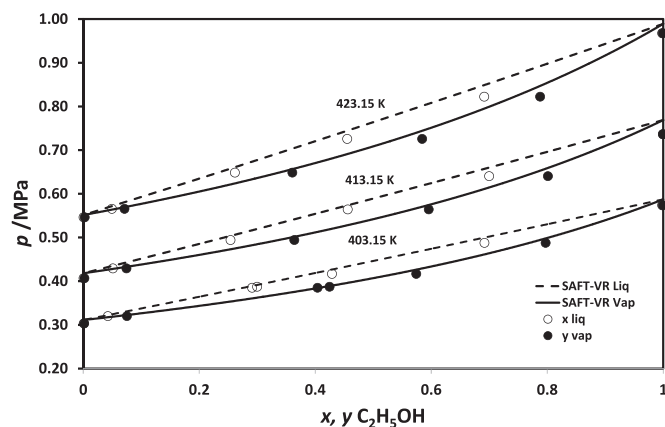


Fig. 1. Comparison between vapour-liquid equilibrium data of present work (● – dew line, ○ – bubble line) and the application of the SAFT-VR theory (–) for ethanol + 1-propanol system at several temperatures, lines.

Table 4

Parameters for the Wagner equation for pure ethanol and 1-propanol obtained by regression from the author's experimental work [6–7] with the work of Ambrose and co-workers [23],[27] and Susial et al. [26].

	<i>T</i> range (K)	<i>A</i>	<i>B</i>	<i>C</i>	<i>D</i>
Ethanol	364.86–513.92	–9.1471	2.3096	–14.2220	138.4619
1-Propanol	383.15–536.71	–8.9697	2.6870	–16.2446	102.2398

pure ethanol-rich mixtures is overestimated, deviating 2.3 to 4.2%. These deviations, however, are of the same order of those found in the literature for the vapour pressure of pure ethanol by different authors, and smaller than the average absolute deviation of the fit from which the model parameters for ethanol were obtained is AAD=6.7% [16]. This is larger than the usual AAD of most pure components fits. This is an additional indication of the relatively high scatter in the experimental vapour-pressure curve of ethanol.

It should be emphasized that in the calculations, the unlike interactions parameters were obtained from Lorentz–Berthelot type combining rules (Eqs. (2–6)), i.e., without recurring to binary interaction parameters. The theoretical results are thus true predictions. The good performance of the Lorentz–Berthelot combining rules reflects the similarity between the two studied substances thus any adjusted binary interaction parameters would be very small.

Although the consistence of VLE data is normally supported by activity coefficients calculations in the liquid phase for mixtures [23], this path was not possible to follow as the liquid mixture is nearly ideal ($\gamma_i \approx 1$), as the data presented in Table 2 can demonstrate. This was expected given the similar chemical nature of the two components. Therefore, an analysis of the quality of the pure fluids vapour pressure data was used instead.

The accurate representation of experimental vapour pressure data over a wide temperature range is usually carried out with multiparameter empirical equations that can be very accurate; here the empirical Wagner equation is used. The Wagner equation (Eqs (7–9)) is one of the best available; it expresses the reduced vapour pressure as a function of reduced temperature [8].

$$\ln p_r^{\text{sat}} = \left(\frac{1}{1 - \tau} \right) (A\tau + B\tau^{1.5} + C\tau^3 + D\tau^6) \quad (7)$$

$$\tau = 1 - T_r = 1 - \frac{T}{T_c} \quad (8)$$

$$p_r^{\text{sat}} = \frac{p^{\text{sat}}}{p_c} \quad (9)$$

where $p_r^{\text{sat}} = p^{\text{sat}}/p_c$ is the reduced saturation vapour pressure, $T_r = T^{\text{sat}}/T_c$ is the reduced saturation temperature, p_c and T_c the critical pressure and temperature, respectively. *A*, *B*, *C* and *D* are fitting coefficients for Eq. (7).

The Wagner equation was applied to our pure component experimental data to obtain the *A*, *B*, *C* and *D* parameters (Table 4). Values of the critical constants for ethanol were used from the new equation of state for ethanol proposed by Schroeder et al. [24], $T_c = 514.71$ K and $p_c = 6.268$ MPa, and for 1-propanol from the work of Gude and Teja [25], $T_c = 536.8$ K and $p_c = 5.17$ MPa. For ethanol the regression data included our experimental data [6] and data of Ambrose et al. [26]. Taking as reference the fitted Wagner equation used here (Eq. (7)), in Fig. 2 the deviations from the experimental vapour pressures data of ethanol from reference [6], Ambrose et al. [26], and the new equation for ethanol recently proposed by Schroeder et al. [24] are shown. It can be seen that our data does not deviate from the fitted equation by more than 15 kPa. The data

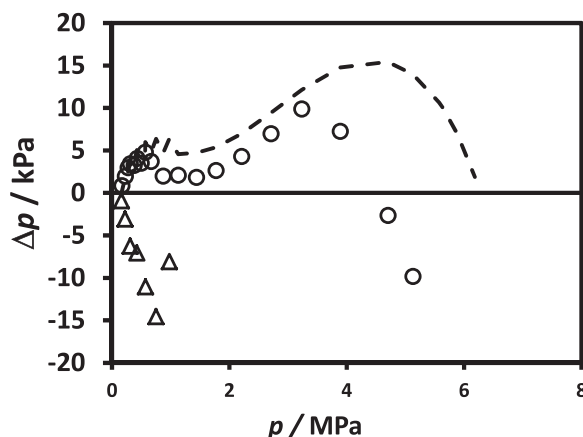


Fig. 2. Deviations from the results of Wagner equation (Eq. (7)) between the experimental vapour pressures data of ethanol from previous paper [6] – Δ , Ambrose [26] – \circ , and from those given by the new equation for ethanol presented by Schroeder et al. [24] – —.

of Ambrose displays deviations of the same magnitude, although of opposite sign, for pressures smaller than 5 MPa diverging to 40 kPa for pressures close to the critical point. Our equation does not deviate from Schroeder et al. data by more than 15 kPa. The paper of Schroeder et al. [24] also presents a modified Wagner equation based on two selected works, by Aucejo et al. [27] and Bazaev et al. [28], and the agreement is rather satisfactory. The agreement of our data with this equation is also remarkably good, within the mutual uncertainty of our experimental data (–20 to +5 kPa) and that calculated by Schroeder et al. [24] (1%) for our pressure range.

The vapour pressure of pure 1-propanol was measured recently by us [7], and it was shown that our data agreed to within their mutual uncertainty with the data of Susial et al. [29]. The Wagner equation was also fitted to our data and to Ambrose and Townsend [30] data. In Fig. 3 the good agreement between these three sets of data in the range of 5 kPa, up to 4 MPa and the Wagner equation now proposed can be appreciated. It is noticeable that as in the case of ethanol, the data of Ambrose diverges up to 40 kPa for pressures closer to the critical pressure.

From these results we can conclude that the new data measured for pure alcohols are consistent with the best experimental data and correlation efforts for both fluids. Furthermore, in terms of the mixture, ideal phase behaviour of the binary mixture of ethanol + 1-propanol is confirmed and the uncertainty of the experimental data is confirmed.

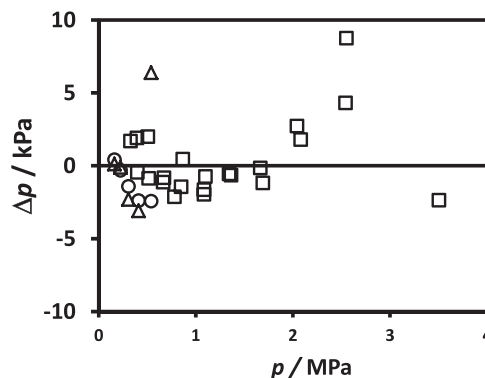


Fig. 3. Deviations from the results of Wagner equation (Eq. (7)) between the experimental vapour pressures data of 1-propanol from previous paper [7] – Δ , Susial et al. [29] – \circ , and Ambrose and Townsend [30] – \square .

5. Conclusion

Experimental VLE data were obtained for the ethanol+1-propanol system for temperatures between 403.2 and 423.2 K, and pressures up to 1 MPa using a flow apparatus.

A coherence test was performed to the pure alcohols vapour pressures using the Wagner equation. The results show a good agreement between our data for the pure alcohols, previous experimental determinations and the recent equation of state of Schroeder et al. for ethanol. The results also show that Wagner equation is as said before one of the most effective in modelling the vapour pressure dependence on temperature. Some minor corrections are known to be necessary to be used near the critical point, where the original exponents of this equation have to be modified, but this is out of scope of present work.

The SAFT-VR theory was used to model the experimental results. The data is quantitatively reproduced without using binary interaction parameters.

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