

## ***p*-*x* data of (acetic acid + water) at *T* = (412.6, 443.2, 483.2) K**

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### **Abstract**

Experimental *p*-*x* data were measured for the (acetic acid + water) system at the temperatures of (412.6, 443.2 and 483.2) K between the pressures of 196 kPa and 1902 kPa over the entire range of concentrations. Experiments were carried out in a static-analytical equipment with quantitative analysis by GC. The experimental data were correlated with the Perturbed-Chain Statistical Associating Fluid Theory considering two association sites for acetic acid and four association sites for water.

### **Keywords**

Vapour liquid equilibria, Acetic acid, Water, PC-SAFT

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## 1 Introduction

Acetic acid and its derivatives are used in several industries making it one of the major worldwide commodity chemicals. The global demand for acetic acid in 2013 was around 10.5 Mt and it is projected to reach 15.5 Mt by 2020 with a market revenue of 12,190 million USD [1,2]. More than 65% of the acetic acid produced in the world ends in the form of polymers, mainly as derivatives of vinyl acetate and cellulose acetate [3]. Other usages include the production of pharmaceuticals (e.g. acetyl salicylic acid) [4], as a reaction solvent of purified terephthalic acid (PTA) for further production of polyethylene terephthalate (PET) [3], and in the food industry, as an acidulant, preservative and flavouring agent [5]. Its most common household usage is in the form of vinegar and as a chemical descaler.

In the two main industrial production processes of acetic acid (oxidation of hydrocarbons and methanol carbonylation [3,6]), water is removed from the crude stream normally by distillation. These, and other processes involving acetic acid aqueous mixtures, require therefore, accurate knowledge of the properties of the phases at equilibrium.

Experimental vapour–liquid equilibria (VLE) data for the system (acetic acid + water) are the most readily available of the carboxylic acids; more than 60 different articles were found in the open literature. The oldest work seems to date back to 1921 [7] while the most recent one to 2012 [8]. Most of the available data are isobaric, the majority are made at sub- and atmospheric conditions. Wichterle, et al. [9,10] and Gmehling and Onken [11] have compiled most of these work. None of the available literature, to our knowledge, have reported azeotropic behaviour of the mixture.

Most of the isothermal data available are at temperatures below 373 K, a temperature below the normal boiling point of acetic acid (391.05 K), mainly because of the corrosive nature of the compounds; the common apparatus for these kind of measurements is made of glass. Special alloys are required to handle the increasing corrosive conditions encountered at higher temperatures. An exemption to the low temperature data is that of Freeman and Wilson [12,13] who presented  $p$ - $x$ - $y$  data at

$T = (372.77, 412.57, 462.06 \text{ and } 502.86) \text{ K}$  and pressures ranging from 56 kPa to 2778 kPa.

In this work, new pressure-composition ( $p$ - $x$ ) data were measured at  $T = (412.6, 443.2 \text{ and } 483.2) \text{ K}$ . The isotherm at 412.6 K from Freeman and Wilson [12] is used for comparison of the new data. Experimental measurements were undertaken using a static-analytical method with sampling of the liquid phase. Concentrations were determined by Gas-Chromatography analysis.

On the other hand, use of a reliable thermodynamic model is necessary for engineering design purposes. In general, use of thermodynamic models in the form of equations of state (EoS) is preferred since these are applicable at a wider range of pressures and since all properties can be derived from the same model. In the case of (acetic acid + water) mixtures, the complex phase behaviour due to molecular interactions such as association must be accounted for in the chosen thermodynamic model.

The Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) [14,15] EoS was selected in this work to model the experimental data since it has been developed to handle association interactions explicitly. In the PC-SAFT framework, the association scheme for the molecules involved has to be defined, for which the classification of Huang and Radosz [16] is commonly used. Based on previous studies [15,17-19] it was decided in this work to model acetic acid with the 2B association scheme, while water with the 4C association scheme. Pure component parameters were refitted in each case. Additionally, the EoS results were compared with those obtained from the UNIQUAC-HOC [20,21] activity coefficient model, where appropriate.

## 2 Experimental

### 2.1 Materials

Table 1 summarizes the chemical compounds used in the experiments as well as their corresponding purities. Gas-Chromatography (GC) analysis of the purchased acetic acid revealed two main peaks, one corresponding to the carboxylic acid while the other

to water in accordance with its hydrophilic characteristics. A third small peak accounting for 0.028% of the mass sample was an unidentified impurity which was considered to be part of the water content. Chemicals were used without further purification and were only subjected to a degassing process as described in Section 2.3.

Table 1. Chemical compounds.

Chemical name	CAS number	Source	Mole fraction purity	Analysis method
acetic acid	64-19-7	Sigma-Aldrich	0.9901	GC <sup>a</sup>
water	7732-18-5	Sigma-Aldrich	1	-

<sup>a</sup> Gas-Chromatography.

## 2.2 Experimental apparatus and uncertainties

The experimental apparatus is described in detail in a previous publication [22]. It consisted mainly of a modified high-pressure vessel made of Hastelloy C (Parr 4575 series) serving as the equilibrium cell with a volume of 250 mL and approximately 17 mm wall thickness; an air-bath (Applied Separations, model Spe-ed SFC) serving as the temperature control environment; a digital pressure gauge (Keller-Druck, model Lex1), range 0 to 2,000 kPa with  $\pm 1$  kPa accuracy according to manufacturer's calibration certificate; T-type thermocouples: one located inside, one at the side and one outside of the equilibrium cell; a thermocouple data logger (Pico Technology, model TC-08) for monitoring and recording temperature; a vacuum pump (KNF Neuberger Edwards, model Laboport PM 13196-840.3); a Hastelloy C internal stirrer; a high-pressure liquid pump (Jasco, model PU-1586) and a GC (Agilent Technologies, model 6850) for quantitative analysis.

The thermocouples were calibrated by comparing measured saturated temperatures of water from  $T = 301$  K to  $T = 487$  K against data from NIST [23]. The equilibrium cell temperature was controlled to within 0.1 K. Combined standard uncertainties in temperature,  $u_c(T)$ , after calibration, control and resolution were  $u_c(T) = 0.1$  K.

Combined standard uncertainties in pressure,  $u_c(p)$ , after considering calibration, repeatability and pressure drop during sampling were estimated as  $u_c(p) = 1$  kPa.

The GC was equipped with a TCD detector and a packed column 3 ft x 1/8" SS Porapak N 80/100 mesh. GC operating conditions were: inlet temperature: 503 K; oven temperature: 423 K, column flow: 40 mL/min (1 min), 60 mL/min (4 min) at 10 mL/min; detector temperature: 473 K; carrier gas: Helium CP grade (BOC, certified purity  $\geq 0.99999$  mole fraction). 0.2  $\mu$ L volume samples were injected with an autosampler. The GC calibration procedure of Raal and Mühlbauer [24] for liquid sample injections was adopted in this work. A linear relationship of area ratio vs. mass fraction ratio was obtained from the low to the high acetic acid concentration regions. Uncertainties in composition are presented for each experimental point in Section 4.

### 2.3 Procedure

The experimental procedure has been described previously [22,25] and is briefly summarized as follows: the equilibrium cell was cleaned thoroughly before each experimental run and subjected to a pressure test with compressed nitrogen. Acetic acid and water were degassed for 1 h in an ultrasonic bath. A mixture of the compounds was loaded into the equilibrium cell and the system was vacuumed down between  $p = 1.5$  kPa and  $p = 2.0$  kPa at room temperature. The desired equilibrium temperature was reached by increasing or decreasing the air bath temperature. The system was allowed to reach equilibrium state under constant stirring, which was assumed when temperature and pressure did not vary within  $\pm 0.05$  K and  $\pm 0.5$  kPa, respectively, for at least 5 min. A minimum of five samples (20  $\mu$ L each) of the liquid phase were withdrawn and collected in 250  $\mu$ L vial inserts. Pressure was increased by adding water into the cell by means of the liquid-pump in order to establish a new experimental point.

### 3 Modelling

PC-SAFT is expressed as the addition of contributions due to hard-chain formation (*hc*), dispersive (*disp*) and association forces (*assoc*) to the residual Helmholtz free energy ( $\hat{a}^{res}$ ) according to ( $\hat{a}^{res}$ ) [15]:

$$\frac{\hat{a}^{res}}{RT} = \frac{\hat{a}^{hc}}{RT} + \frac{\hat{a}^{disp}}{RT} + \frac{\hat{a}^{assoc}}{RT} \quad (1)$$

The compressibility factor is then expressed by:

$$Z = 1 + Z^{hc} + Z^{disp} + Z^{assoc} \quad (2)$$

The five pure component parameters needed to characterize a pure component are: the number of segments per chain ( $m$ ), the segment diameter ( $\sigma$ ), the depth of the pair potential ( $\varepsilon$ ), the association energy ( $\varepsilon^{A_i B_i}$ ) and the association volume ( $\kappa^{A_i B_i}$ ). For mixtures, conventional combining rules for  $\sigma$  and  $\varepsilon$  are used:

$$\sigma_{ij} = \frac{(\sigma_i + \sigma_j)}{2} \quad (3)$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j} (1 - k_{ij}) \quad (4)$$

where  $k_{ij}$  is the binary interaction parameter. Wolbach and Sandler [15] combining rules were used for the cross-association interactions:

$$\varepsilon^{A_i B_j} = \frac{\varepsilon^{A_i B_i} + \varepsilon^{A_j B_j}}{2} \quad (5)$$

$$\kappa^{A_i B_j} = \sqrt{\kappa^{A_i B_i} \kappa^{A_j B_j}} \left( \frac{\sqrt{\sigma_i \sigma_j}}{(\sigma_i + \sigma_j)/2} \right)^3 \quad (6)$$

Pure component parameters were obtained by fitting vapour pressure ( $p_v$ ) and liquid density ( $\rho_v$ ) data simultaneously with the procedure described in a previous publication [22], with the following objective function:

$$F_1 = \sum_{i=1}^N \left[ \left( \frac{p_{V,i}^{exp} - p_{V,i}^{calc}}{p_{V,i}^{exp}} \right)^2 \left( \frac{\rho_{L,i}^{exp} - \rho_{L,i}^{calc}}{\rho_{L,i}^{exp}} \right)^2 \right] \quad (7)$$

where *exp* and *calc* stand for an experimental and a calculated property, respectively; and  $N$  is the number of experimental points used in the optimization.

The optimum  $k_{ij}$  was obtained by regressing the experimental bubble point pressures ( $p$ ) with Eq. (8) as the objective function:

$$F_2 = \sum_{i=1}^N \left( \frac{p_i^{exp} - p_i^{calc}}{p_i^{exp}} \right)^2 \quad (8)$$

## 4 Results and Discussion

### 4.1 Experimental

The experimental  $p$ - $x$  data obtained at  $T = (412.6, 443.2 \text{ and } 483.2)$  K as well as the uncertainties in composition are shown in Table 2. Relative errors in the measured water vapour pressures against reference data from NIST [23] were: 0.07, 0.12, and 0.40% at  $T = (412.6, 443.2 \text{ and } 483.2)$  K, respectively.

A yellow-greenish colour liquid remained at the end of the experimental runs evidencing corrosion. A more intense colour was observed at the maximum run temperature of 483.2 K for a concentrated mixture of organic acid, for which a 0.01% iron content was determined by spectrophotometry. Othmer, et al. [26] have shown in

their studies of (acetic acid + water) in a Type SS-316 still that a presence of 2% content gave no interference to the phase behaviour when testing a 85 wt.% acetic acid solution at  $T = 503$  K and  $p = 2.17$  MPa.

Table 2. Experimental equilibrium data for the {acetic acid (1) + water (2)} system at pressure  $p$ , liquid mole fraction  $x$  and temperatures  $T = (413.2, 443.2$  and  $483.2)$  K.<sup>a</sup>

$T = 412.6$ K			$T = 443.2$ K			$T = 483.2$ K		
$p/\text{kPa}$	$x_1$	$u_c(x_1)$	$p/\text{kPa}$	$x_1$	$u_c(x_1)$	$p/\text{kPa}$	$x_1$	$u_c(x_1)$
196	0.976	0.005	426	0.983	0.005	1012	0.977	0.005
210	0.951	0.005	437	0.975	0.005	1052	0.955	0.005
230	0.889	0.005	461	0.955	0.005	1150	0.895	0.005
266	0.721	0.005	504	0.903	0.005	1272	0.822	0.005
290	0.579	0.005	551	0.823	0.008	1401	0.689	0.005
311	0.433	0.005	605	0.697	0.005	1515	0.580	0.005
326	0.347	0.005	654	0.568	0.001	1652	0.444	0.005
333	0.282	0.005	704	0.409	0.003	1690	0.407	0.005
341	0.186	0.005	731	0.315	0.001	1750	0.335	0.005
348	0.102	0.010	760	0.195	0.005	1796	0.275	0.005
349	0.085	0.005	768	0.178	0.005	1821	0.234	0.005
353	0.014	0.005	774	0.148	0.005	1855	0.178	0.005
356	0.000		780	0.133	0.005	1870	0.153	0.005
			786	0.105	0.005	1881	0.100	0.005
			789	0.055	0.005	1890	0.078	0.005
			792	0.000		1896	0.048	0.005
						1900	0.034	0.005
						1902	0.000	

<sup>a</sup> Combined standard uncertainties,  $u_c$ , are  $u_c(T) = 0.1$  K,  $u_c(p) = 1$  kPa.  $u_c(x)$  are displayed in each temperature column.

## 4.2 Modelling

The pure component parameters for both compounds are presented in Table 3, with acetic acid and water modelled as a 2B and a 4C association molecule, respectively. The effect of different parameters for water on the modelling has been discussed before [27].

Table 3. PC-SAFT pure component parameters and average deviations in vapour pressures ( $\Delta p_v$ ) and liquid densities ( $\Delta \rho_L$ ).<sup>a, b</sup>

Compound	$m$	$\sigma/\text{\AA}$	$\varepsilon/k/K$	$\kappa^{A_i B_i}$	$\varepsilon^{A_i B_i}/\kappa/K$	$T^c/K$	$\Delta p_v^d/\%$	$\Delta \rho_L^d/\%$
acetic acid	2.5969	3.0474	190.22	0.368320	2379.0	290 – 586	0.83	0.96
water	3.0639	1.9701	150.10	0.429973	1523.7	273 – 640	0.75	2.00

<sup>a</sup> Vapour pressure and liquid density data taken from DIPPR [28].

<sup>b</sup> Acetic acid and water modelled as 2B and 4C association type, respectively.

<sup>c</sup> Temperature range used in the optimization.



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$$^d \Delta\theta = \frac{100}{N} \sum_{i=1}^N \left| \frac{\theta^{exp} - \theta^{calc}}{\theta^{exp}} \right|, \text{ for } \theta \text{ either } p_v \text{ or } \rho_L.$$

The adjusted  $k_{ij}$  were -0.0099, -0.0012 and -0.0016 for the (412.6, 443.2 and 483.2) K isotherms, respectively. These values are one order of magnitude lower than the ones reported in previous publications [18,19].

Figure 1 shows a comparison of the new data against those of the literature values of Freeman and Wilson [12] at  $T = 412.6$  K. Both data sources for the liquid compositions agree relatively well. It is necessary, however, to point out some aspects of the literature values. They exhibit a maximum pressure of  $p = 359$  kPa in the dilute acetic acid region after which the pressure decreases sharply, reaching a water vapour pressure of 350.2 kPa. There is no obvious reason for this maximum to happen. It is likely that repeatability was not easy to achieve because of thermal and composition gradients not eliminated due to the lack of stirring. It is reasonable to assume that deviations in pressure must be larger than the reported ones since the stated vapour pressure of water at 412.6 K gives a relative error of 1.6% (NIST data as reference) in contrast to that of 0.07% of this work. One can conclude that the experimental values of the liquid compositions obtained in the present work are more reliable than those reported by the previous authors, although the accuracy reported in the literature is actually lower ( $u_c(x_1) = 0.001$  vs. an average of  $u_c(x_1) = 0.005$  in this work).

Figure 1 also presents the modelling results with PC-SAFT, and as a comparison, modelling with the UNIQUAC [20] activity coefficient coupled with the Hayden-O'Connell term [21] (UNIQUAC-HOC), which considers the non-idealities of the vapour phase of organic acids, is presented as well. The following default pure compound and binary interaction parameters were used in the UNIQUAC-HOC model: association parameter ( $\eta$ ) = 4.5, 1.7 and 2.5 for the acetic acid, water and cross-interactions, respectively;  $a_{ij} = 0.7446$ ,  $a_{ji} = 0.0042$ ,  $b_{ij} = -615.264$  and  $b_{ji} = 196.899$ . As can be seen, in general the liquid phase concentrations are better correlated by PC-SAFT, even in the dilute acetic acid region (Figure 2) with the exception of the concentrations of  $x_1 < 0.014$ .

The isotherms at 443.2 K and 483.2 K are presented in Figures 3 and 4, respectively. It can be observed that PC-SAFT can correlate satisfactorily the bubble pressures at both temperatures.

As an additional plot, the isotherm reported by Freeman and Wilson [12] at  $T = 502.85$  K is presented in Figure 5. PC-SAFT is able to model accurately the compositions of both phases with  $k_{ij} = -0.012$ .

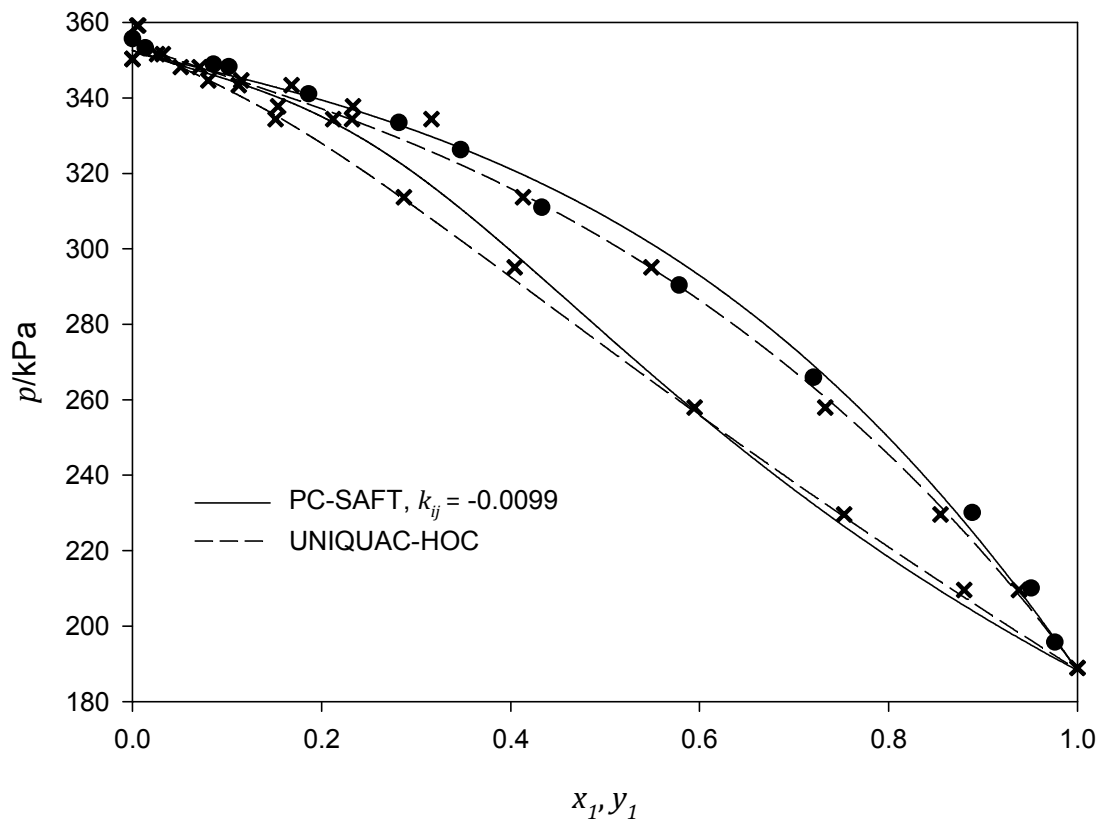


Figure 1. Vapour–liquid equilibrium diagram for the {acetic acid (1) + water (2)} system at  $T = 412.6$  K. Experimental data: (x) Freeman and Wilson [12]; (●) this work.

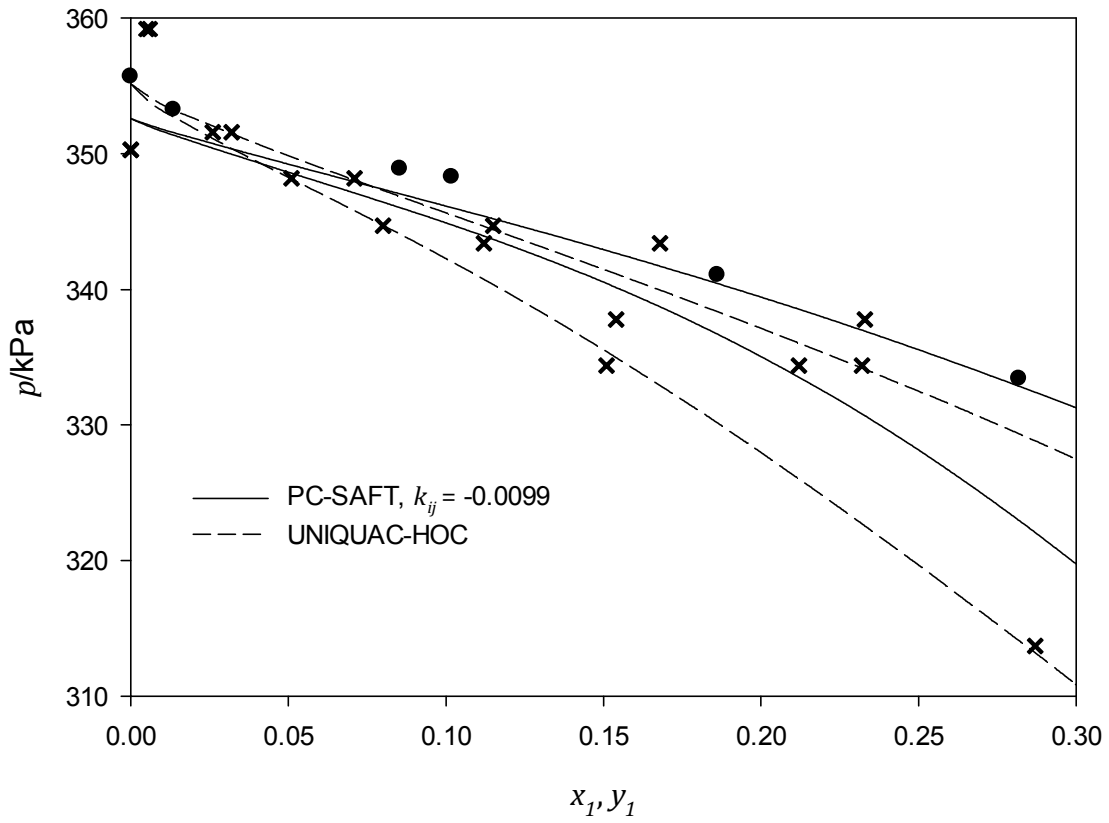


Figure 2. Vapour–liquid equilibrium diagram for the {acetic acid (1) + water (2)} system in the  $x_1 = (0 \text{ to } 0.3)$  region at  $T = 412.6 \text{ K}$ . Experimental data: (x) Freeman and Wilson [12]; (•) this work.

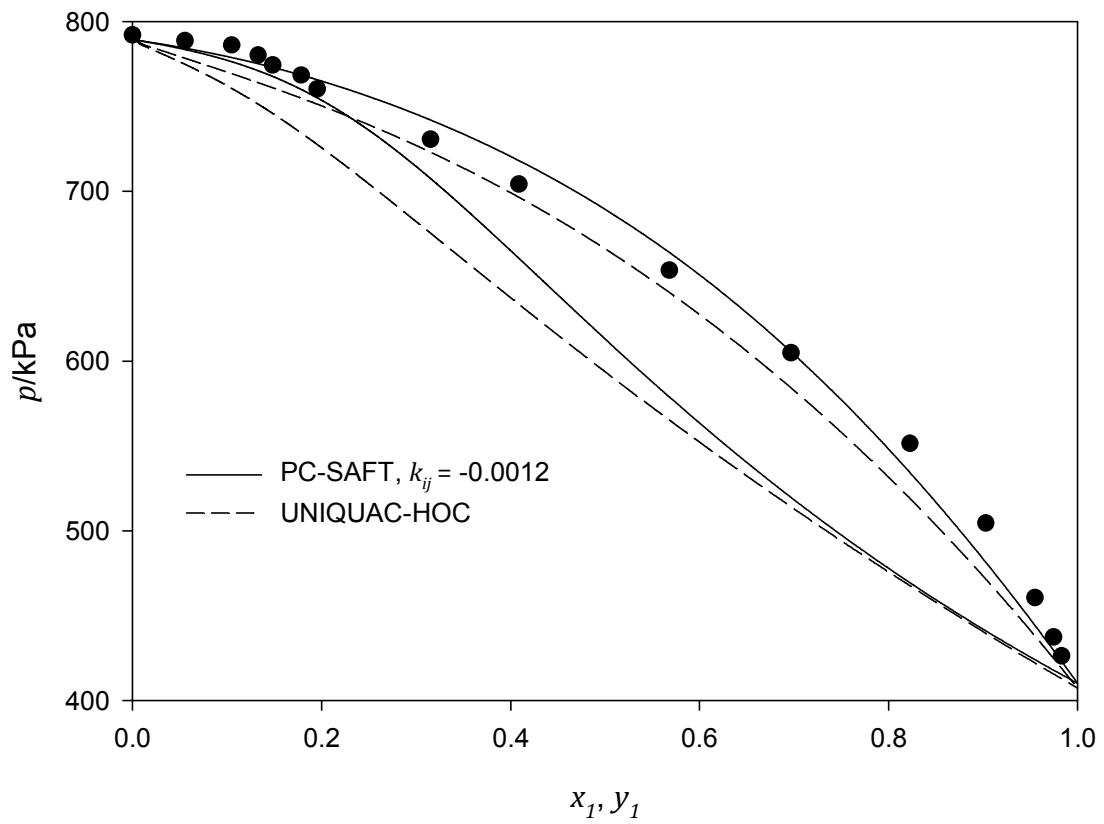


Figure 3. Vapour–liquid equilibrium diagram for the {acetic acid (1) + water (2)} system at  $T = 443.2$  K. Symbols: experimental data from this work.

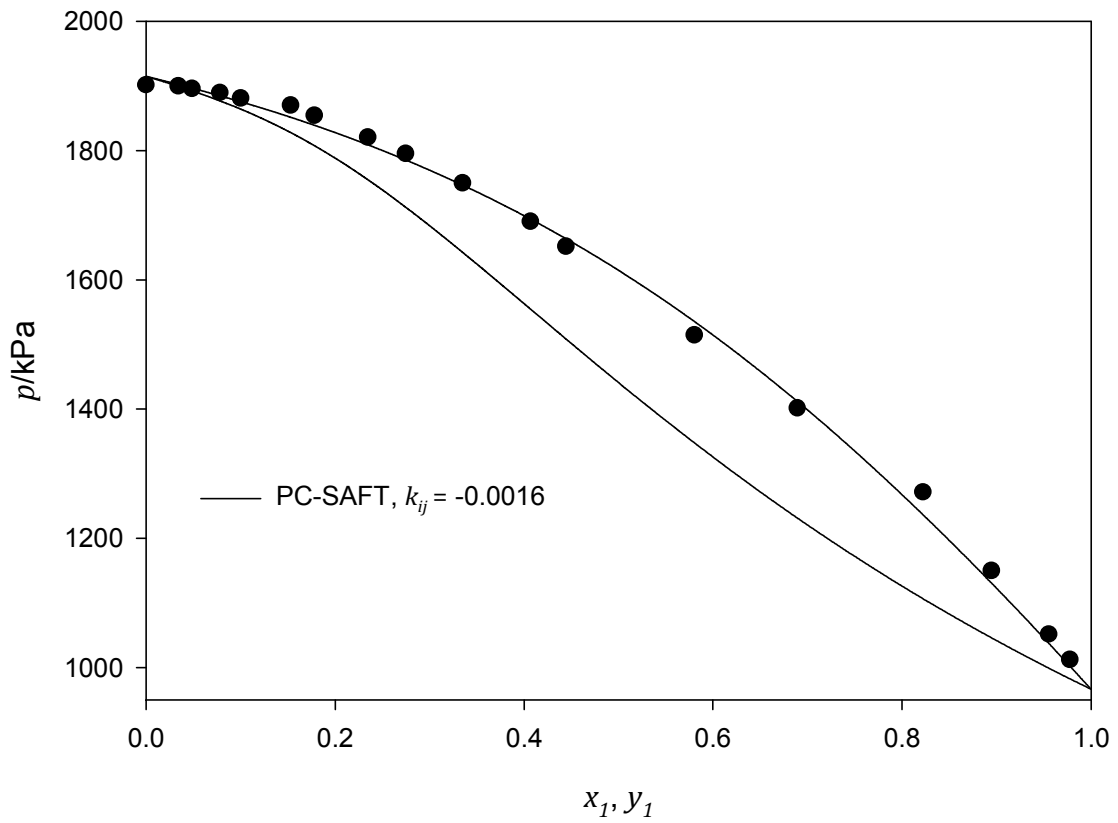


Figure 4. Vapour–liquid equilibrium diagram for the {acetic acid (1) + water (2)} system at  $T = 483.2$  K. Symbols: experimental data from this work.

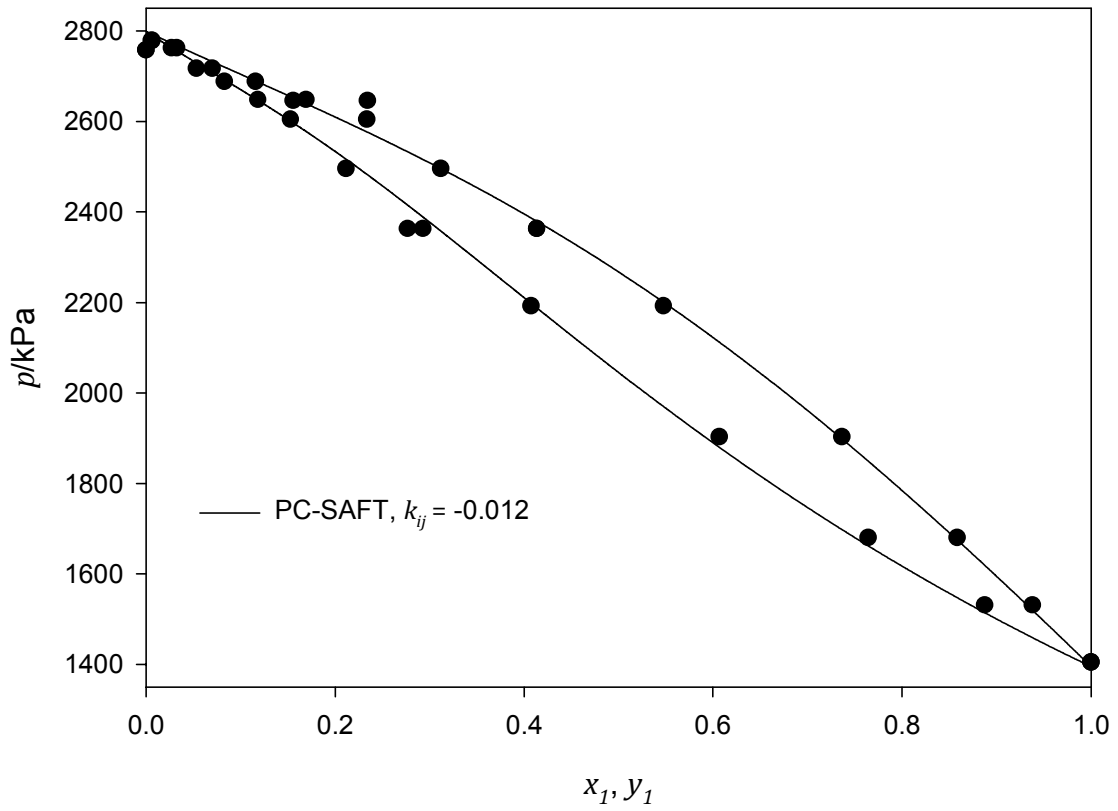


Figure 5. Vapour–liquid equilibrium diagram for the {acetic acid (1) + water (2)} system at  $T = 502.85$  K. Symbols: experimental data from Freeman and Wilson [12].

## 5 Conclusions

Experimental pressures and liquid phase compositions were measured for the (acetic acid + water) system at the temperatures of (412.6, 443.2 and 483.2) K. PC-SAFT, with water modelled as a 2B and acetic acid as a 4C association molecule, was able to correlate satisfactorily the experimental data including high-pressure data. New pure component parameters for acetic acid and water are presented for the corresponding association schemes.

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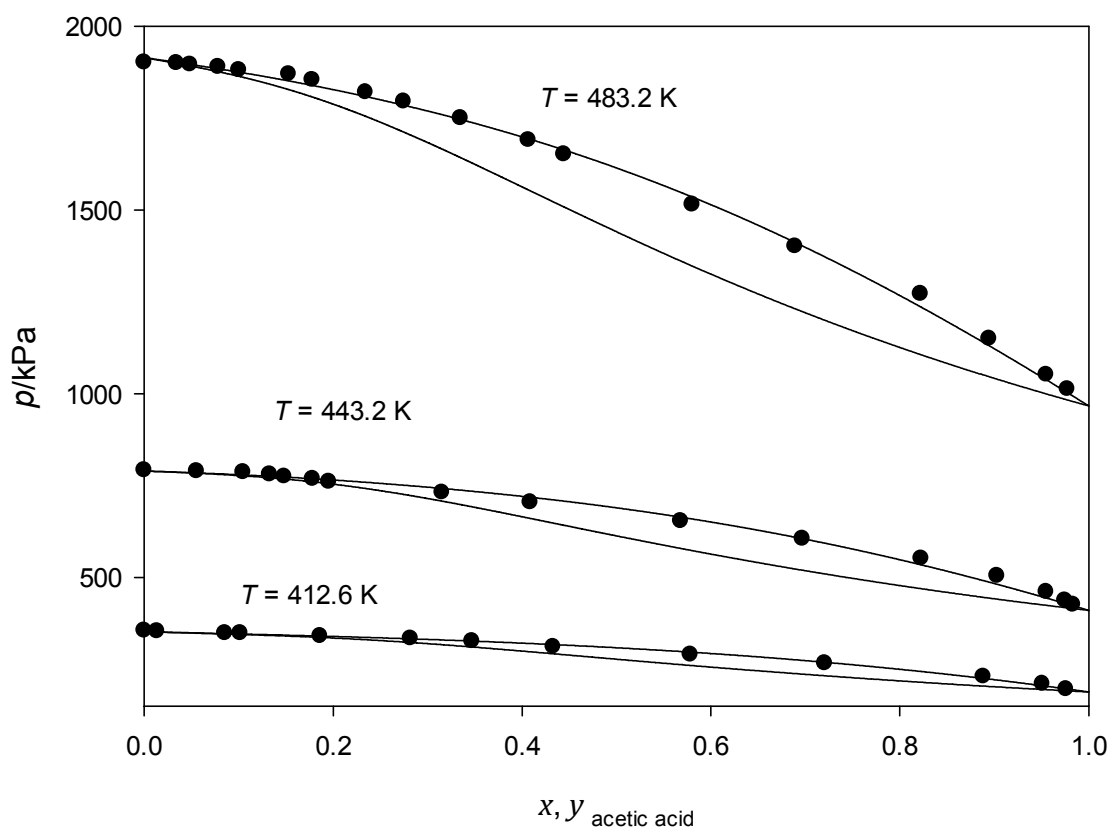
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$p$ - $x$  data of (acetic acid + water) at  $T = (412.6, 443.2, 483.2) \text{ K}$ .

Luis A. Román-Ramírez

Gary A. Leeke

# p–x Data of (Acetic Acid + Water) at T = (412.6, 443.2, 483.2) K

Roman-Ramirez, Luis A.

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