Compressed and Saturated Liquid Densities for the 2-Propanol + Water System

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Compressed liquid densities for the 2-propanol (1) + water (2) mixture have been determined at (300, 325, and 350) K and x_1 close to 0.25, 0.49, and 0.73 using a vibrating tube densimeter. Liquid densities have been measured from about atmospheric pressure up to 10 MPa and correlated with a multilayer feedforward neural network. The composition dependence of the excess molar volume has been evaluated in the temperature and pressure range of the experimental data. A model based on a multilayer feedforward neural network function combined with the saturated pressure equation of the pure fluids has been regressed on the available literature data for the bubble pressure. The correlations for liquid density and bubble pressure have been used to generate the saturated liquid density surface in the whole temperature range of the measured compressed liquid densities and for compositions ranging from the pure 2-propanol to the pure water.

1. Introduction

This paper is a continuing effort to study alternative methods compatible with the requirements of sustainable development, environmental impact, and energy saving.[1,2] A recent paper has addressed the study of the propylene + 2-propanol mixture,[2] while a further one will be published for the study of the ternary mixture propylene + 2-propanol + water.[3]

The literature reports a number of experimental works about measurements of the liquid density and vapor−liquid equilibria of the 2-propanol + water mixture with which the original data presented in the following will be compared. In particular, the sources in the range of interest for the density are from ref 11 to ref 23, while for the bubble pressure, the sources from ref 24 to ref 34 are assumed for the definition of the saturated liquid condition. The "synthetic open circuit method" taking advantage of a vibrating tube densimeter (VTD)[2] was used.

The obtained liquid density values have been correlated using a multilayer feedforward neural network (MLFN) function. The produced model has been used to study the composition dependence of the excess volumes at constant temperature and pressure.

A bubble pressure model combining a MLFN and saturated pressure equations for the pure fluids was obtained correlating the literature bubble pressures for the 2-propanol (1) + water (2) mixture in the (298 to 374) K temperature range.

The saturated liquid density surface in the whole composition range and for temperatures ranging from (287 to 350) K has been obtained as an intersection of the model regressed on single-phase liquid densities and the model regressed on bubble pressures.

2. Experimental

2.1. Chemicals. The 2-propanol (molar mass = 60.096 kg·kmol^{-1}, CAS Number 67-63-0) is from Sigma-Aldrich with a GC certified purity higher than 99.8 %. Ultrapure water is produced with a Direct-Q model from Millipore. Both 2-propanol and water were carefully degassed before use.

2.2. Apparatus and Experimental Procedure. A detailed description of the apparatus is given in ref 4, and its schematic layout is presented in ref 2. The apparatus employs synthetic mixtures that have been prepared gravimetrically under vacuum according to the procedures presented in ref 5.

Readers are encouraged to look for details about the experimental procedure in ref 2.

2.3. Experimental Uncertainties. The experimental uncertainties have been calculated taking into account the expanded uncertainties and coverage factor as described in ref 6. The period of vibration is converted into density using the forced path mechanical calibration (FPMC).[7]The first reference for the calibration is the period of vibration measured at vacuum conditions, while the second reference is the period of vibration measured with the refrigerant R134a. For both the references, measurements have been carried out at the same temperature and in the same pressure range of the target mixture (see ref 7).

The global uncertainty on density data in the liquid phase is estimated to be within 0.05 %. The uncertainty on vibrating period values is $\pm 10^{-8}$ s. Global temperature uncertainties are estimated to be about ± 0.02 K with a confidence level of approximately 68 %. Global uncertainties on pressure measurement are ± 0.0001 MPa (for $0 < P \leq 0.6$ MPa) and ± 0.0006 MPa (for $0.6 < P \leq 10.6$ MPa) with a confidence level of approximately 68 %. Uncertainties in mixture composition are within $2 \cdot 10^{-4}$ in molar fraction.

3. Experimental Results

The liquid density measurements for the 2-propanol (1) + water (2) mixture have been carried out at (300, 325, and 350) K from 10 MPa down to about atmospheric pressure for the $x_1 = 0.25$, 0.49, and 0.73 molar fractions. The measured (P, ρ, T, $\bar{x}$) values are reported in Table 1. In Figure 1, the measured data are shown together with liquid density values of pure 2-propanol[8] and water[9] at the same temperatures of the mixture measurements and for pressures ranging from the pure fluid bubble points up to 10 MPa.

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Table 1. Experimental Liquid Density Data for the 2-Propanol (1) + Water (2) Mixture

$x_1 = 0.2483$

$T = 300.08$ K		$T = 325.10$ K		$T = 350.18$ K	
P/MPa	ρ/kg·m^{-3}	P/MPa	ρ/kg·m^{-3}	P/MPa	ρ/kg·m^{-3}
0.1462	895.50	0.0726	874.13	0.2200	850.33
0.3813	895.67	0.4103	874.37	0.5110	850.54
0.7649	895.89	0.9621	874.71	0.9388	850.91
1.1011	896.11	1.3430	875.01	1.3697	851.29
1.5568	896.32	1.8595	875.37	2.0669	851.75
1.9219	896.56	2.3326	875.60	2.3810	852.09
2.1815	896.86	2.8264	875.91	2.7181	852.39
2.6101	897.09	3.3194	876.24	3.1077	852.73
3.0805	897.32	3.7763	876.52	3.4648	853.04
3.5223	897.58	4.2367	876.83	3.9576	853.37
4.0826	897.87	4.5987	877.08	4.3460	853.71
4.6633	898.17	5.0893	877.36	4.7811	854.06
5.1513	898.42	5.5642	877.68	5.2678	854.49
5.5625	898.65	5.9542	877.93	5.7438	854.83
5.9805	898.85	6.3943	878.21	6.1964	855.20
6.4143	899.11	6.8085	878.48	6.7342	855.63
6.7548	899.33	7.2880	878.80	7.3749	856.07
7.2468	899.56	7.7827	879.08	7.9990	856.54
7.6367	899.78	8.0791	879.34	8.6303	857.02
8.1316	900.04	8.4389	879.63	9.2983	857.54
8.6628	900.28	8.8285	879.87		
9.0873	900.54	9.3589	880.18		
9.5623	900.79				

$x_1 = 0.4939$

$T = 300.10$ K		$T = 325.09$ K		$T = 350.15$ K	
P/MPa	ρ/kg·m^{-3}	P/MPa	ρ/kg·m^{-3}	P/MPa	ρ/kg·m^{-3}
0.2334	838.18	0.0654	814.96	0.1617	789.80
0.5030	838.33	0.3030	815.20	0.3878	790.10
0.9466	838.71	0.6453	815.47	0.6952	790.45
1.5453	839.06	1.0048	815.80	1.0208	790.78
1.9022	839.36	1.3919	816.13	1.4001	791.25
2.3035	839.65	1.7881	816.48	1.7958	791.61
2.7246	839.96	2.2420	816.83	2.1471	791.96
3.1365	840.26	2.8811	817.33	2.4979	792.31
3.5679	840.56	3.9046	818.19	2.8927	792.74
3.9958	840.87	4.2421	818.51	3.2779	793.12
4.4362	841.18	4.7844	818.94	3.6115	793.50
4.8355	841.48	5.1168	819.26	4.0873	794.01
5.2620	841.77	5.5073	819.61	4.6067	794.49
5.6998	842.07	5.9122	819.93	4.9552	794.83
6.1610	842.39	6.3221	820.28	5.3760	795.26
6.5884	842.68	6.7730	820.60	5.8376	795.69
7.0530	843.00	7.2145	820.97	6.2964	796.18
7.4379	843.28	7.6133	821.31	6.8866	796.77
7.8620	843.57	8.0805	821.70	7.4008	797.28
8.2485	843.86	8.6031	822.11	7.9356	797.73
8.7044	844.15	9.1973	822.51	8.4003	798.24
9.2606	844.49	9.5614	822.86	9.0006	798.68
9.9664	845.04			9.5212	799.18

$x_1 = 0.7258$

$T = 300.08$ K		$T = 325.13$ K		$T = 351.14$ K	
P/MPa	ρ/kg·m^{-3}	P/MPa	ρ/kg·m^{-3}	P/MPa	ρ/kg·m^{-3}
0.0882	805.57	0.0830	782.69	0.2415	757.15
0.3030	805.78	0.2681	782.93	0.4445	757.34
0.5651	806.00	0.5283	783.18	0.8224	757.80
1.1262	806.42	0.8737	783.50	1.2716	758.33
1.7025	806.92	1.2986	783.92	1.6739	758.75
2.2398	807.33	1.7092	784.33	2.0705	759.26
2.7227	807.73	2.2007	784.79	2.4611	759.66
3.1960	808.11	2.6521	785.22	2.8634	760.12
3.7156	808.53	3.1017	785.67	3.2809	760.61
4.2315	808.93	3.5506	786.11	4.2525	761.65
4.5871	809.31	4.0683	786.61	4.6264	762.11
5.3146	809.85	4.5794	787.07	5.0759	762.61
5.7932	810.24	5.0217	787.49	5.5585	763.09
6.3012	810.63	5.4961	787.93	5.9762	763.59
6.7839	811.02	5.9723	788.38	6.4398	764.08
7.2976	811.43	6.4508	788.82	6.8822	764.57
7.8044	811.81	6.9030	789.24	7.3486	765.10
8.3422	812.23	7.3920	789.70	7.8093	765.60
8.8180	812.60	7.8611	790.11	8.2540	766.09
9.3301	813.00	8.3228	790.52	8.7202	766.63
9.9189	813.45	8.8139	790.98	9.2213	767.15
		9.2874	791.41	9.7148	767.73
		9.8297	791.93	10.2395	768.31

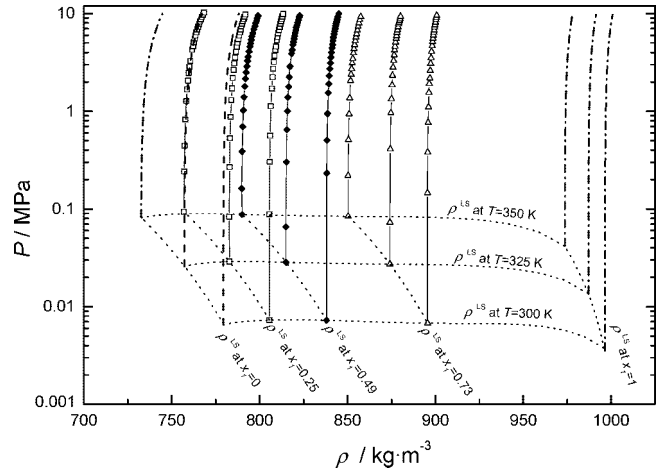

Figure 1. Liquid density measurements for the 2-propanol (1) + water (2) mixture.

The temperature dependence at constant composition of the 2-propanol (1) + water (2) mixture is shown in Figure 2a, while the composition dependence at constant temperature is shown in Figure 2b. In Figures 1 and 2, the dotted lines represent saturated liquid densities ρ^{SL} obtained through the models presented in the following section 4.

4. Modeling Methods

4.1. General Features of the Multilayer Feedforward Neural Network. Multilayer feedforward neural network (MLFN) functional forms have been used to correlate experimental values for the compressed liquid density and literature values for the bubble pressure. The general architecture of an MLFN, as illustrated in Figure 3, is composed of a certain number of units, called *neurons*, organized in three layers called the *input*, *hidden*, and *output* layers, respectively. The neurons of the input layer are indicated as elements of an array $\bar{U}$ of dimension I. Their number coincides with the number of independent variables of the equation plus one. The last neuron, labeled bias 1, has a constant value

$$U_I = \text{bias 1} \tag{1}$$

The number of neurons of the output layer equals the output quantities, which are elements of an array $\bar{S}$ of dimension K.

The hidden layer performs the transformation of the signals from the input layer to the output layer, and it can contain an arbitrary number of neurons. These are elements of an array $\bar{H}$ of dimension $J + 1$. Also in the hidden layer, there is a bias neuron with a constant value, bias 2

$$H_{J+1} = \text{bias 2} \tag{2}$$

The physical input variables V_i (temperature, pressure, and mole fraction for the liquid density correlation and temperature and composition for the bubble pressure correlation) undergo a linear transformation to normalize them in the arbitrarily chosen range $[A_{\min}, A_{\max}]$ set as $A_{\min} = 0.05$ and $A_{\max} = 0.95$

$$U_i = u_i(V_i - V_{i,\min}) + A_{\min} \quad \text{for} \quad 1 \le i \le I - 1 \tag{3}$$

where

$$u_i = \frac{A_{\max} - A_{\min}}{V_{i,\max} - V_{i,\min}} \tag{4}$$

and $V_{i,\min}$ and $V_{i,\max}$ represent the selected extremes of the range of the variable V_i.

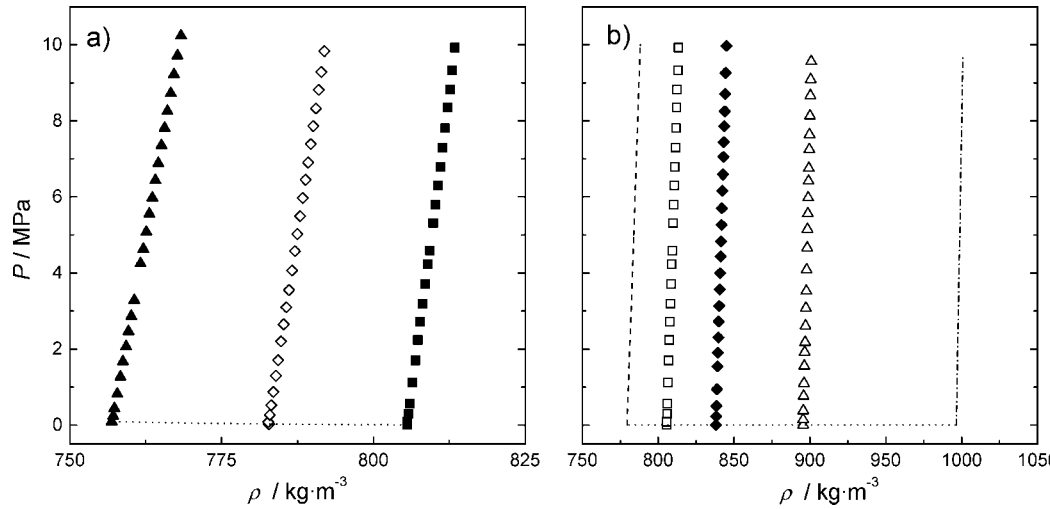

Figure 2. Liquid density measurements for the 2-propanol (1) + water (2) mixture. (a) Temperature dependence at constant composition ($x_1 = 0.73$): ■, 300 K; ◇, 325 K; ▲, 351 K. (b) Composition dependence at constant temperature ($T = 300$ K): □, $x_1 = 0.73$; ◆, $x_1 = 0.49$; △, $x_1 = 0.25$; ••••, ρ^{SL}; - - -, 2-propanol; •-•-•-, water.

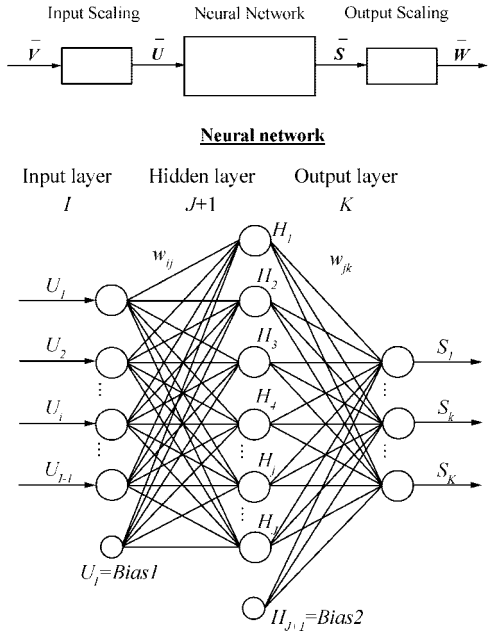

Figure 3. General topology of a three-layer feedforward neural network.

The transfer function, $g(z)$, calculates the signal output of a neuron from its inputs for both the hidden and the output layer neurons. Respectively, it is

$$H_j = g\left(\sum_{i=1}^{I} w_{ij} U_i\right) \quad \text{for} \quad 1 \le j \le J \tag{5}$$

$$S_k = g\left(\sum_{j=1}^{J+1} w_{jk} H_j\right) \quad \text{for} \quad 1 \le k \le K \tag{6}$$

The symbols w_{ij} and w_{jk} indicate the *weighting factors* that are the free parameters of the model, which must be determined by the regression process. The output values S_k of the output layer neurons are denormalized to real output variables W_k, which are in this case the scale factors f_m and h_m, through the following linear transformation

$$W_k = \frac{S_k - A_{\min}}{s_k} + W_{k,\min} \quad \text{for} \quad 1 \le k \le K \tag{7}$$

where

$$s_k = \frac{A_{\max} - A_{\min}}{W_{k,\max} - W_{k,\min}} \tag{8}$$

Table 2. Parameters of the Feedforward Neural Network Used in Equation 9 for the Correlation of the Liquid Density Data of the 2-Propanol (1) + Water (2) Mixture

$\beta = 0.5$			$V_{\min,1} = T_{\min} = 250$			$V_{\max,1} = T_{\max} = 600$		
$I = 4$			$V_{\min,2} = P_{\min} = 0$			$V_{\max,2} = P_{\max} = 200$		
$J = 6$			$V_{\min,3} = x_{\min} = 0$			$V_{\max,3} = x_{\max} = 1$		
$K = 1$			$W_{\min,1} = \rho_{\min} = 650$			$W_{\max,1} = \rho_{\max} = 1050$		
i	j	w_{ij}	i	j	w_{ij}	j	k	w_{jk}
1	1	$-9.31363 \cdot 10^{-1}$	3	1	$-7.46161 \cdot 10^{-1}$	1	1	$1.40240 \cdot 10^{1}$
1	2	1.90004	3	2	8.78966	2	1	$-1.04466 \cdot 10^{1}$
1	3	−2.65487	3	3	5.07904	3	1	−3.93483
1	4	−7.11414	3	4	−1.29070	4	1	8.77578
1	5	$4.42480 \cdot 10^{-1}$	3	5	2.27958	5	1	2.06857
1	6	$-1.37567 \cdot 10^{1}$	3	6	$-1.41375 \cdot 10^{1}$	6	1	$-1.23929 \cdot 10^{1}$
2	1	$2.02051 \cdot 10^{-1}$	4	1	$-3.92838 \cdot 10^{-1}$	7	1	$9.84349 \cdot 10^{-1}$
2	2	−1.45314	4	2	1.95147			
2	3	2.17204	4	3	2.13417			
2	4	5.91087	4	4	6.00562			
2	5	$9.04961 \cdot 10^{-1}$	4	5	−2.26466			
2	6	−3.85432	4	6	−1.12442			

Table 3. Accuracy of the Feedforward Neural Network Model, Equation 9, in the Representation of the Liquid Density Data of the 2-Propanol (1) + Water (2) Mixture

system	ref	NPT[a]	T range (K)	P range (MPa)	x_1 range	AAD (%)	bias (%)	MAD (%)
			training data					
binary mixture	this work	200	300 to 350	0.07 to 10.24	0.25 to 0.73	0.003	0.000	0.012
2-propanol	Stringari et al.[8]	123	300 to 350	0.01 to 0.00	1.00	0.016	0.004	0.030
water	Wagner and Pruβ (DEoS)[9]	120	300 to 350	0.00 to 9.75	0.00	0.011	0.009	0.035
		443	300 to 350	0.00 to 10.24	0.00 to 1.00	0.009	0.004	0.035
			validation data					
binary mixture	Grigiante et al.[11]	15	288 to 308	0.10	0.25 to 0.74	0.011	−0.006	0.026
binary mixture	Egorov et al.[12]	70	288 to 338	0.10	0.00 to 1.00	0.066	0.010	0.283
binary mixture	Hynčica et al.[13]	55	298 to 338	0.39 to 0.50	0.00 to 0.01	0.058	−0.058	0.150
binary mixture	Origlia-Luster and Woolley[14]	72	288 to 358	0.35	0.00 to 0.02	0.052	−0.048	0.208
binary mixture	Arce et al.[15]	19	298	0.10	0.07 to 0.95	0.035	0.017	0.120
binary mixture	Boned et al.[16]	81	303 to 343	0.10 to 10.00	0.10 to 0.90	0.071	−0.060	0.219
binary mixture	Schulte et al.[17]	9	302	0.10	0.00 to 0.02	0.086	−0.086	0.159
binary mixture	Rauf et al.[18]	27	298 to 308	0.10	0.03 to 0.85	0.279	0.242	0.687
binary mixture	Sakurai[19]	292	288 to 318	0.10	0.00 to 1.00	0.063	−0.028	0.274
binary mixture	Kubota et al.[20]	11	298 to 348	0.10	0.06 to 0.75	0.050	0.010	0.173
binary mixture	Høiland[21]	14	293 to 298	0.10	0.00 to 0.01	0.050	−0.033	0.11
binary mixture	Roux et al.[22]	14	298	0.10	0.01 to 0.76	0.156	0.027	0.691
binary mixture	Friedman and Scheraga[23]	15	293 to 323	0.10	0.00 to 0.01	0.028	−0.026	0.058
		1137	288 to 350	0.00 to 10.24	0.00 to 1.00	0.046	−0.010	0.691

[a] NPT: number of experimental points.

$W_{k,\min}$ and $W_{k,\max}$ are chosen limits for the range of the dependent variable W_k.

4.2. Compressed Liquid Density Model. Compressed liquid density as a function of temperature, pressure, and composition has been represented using a simple MLFN model

$$\rho(T, P, x_1) = W_1 \tag{9}$$

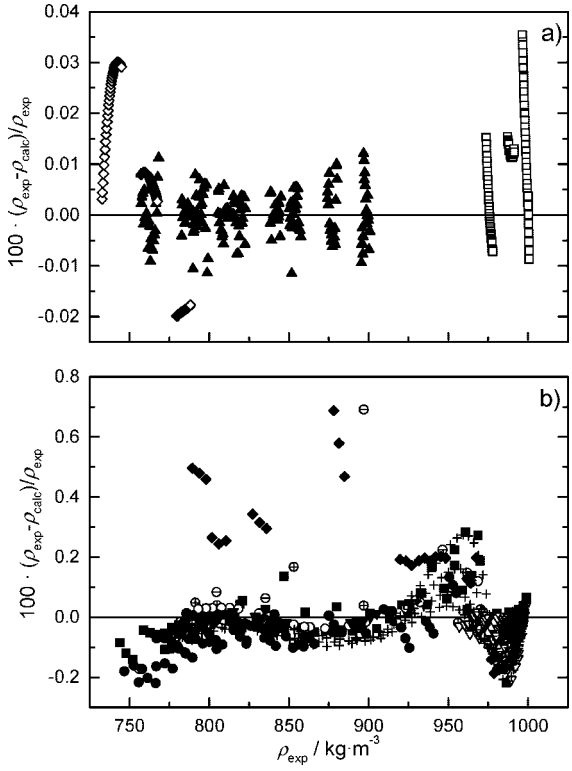

Figure 4. Percentage deviation of the feedforward neural network model, eq 9, in the representation of the liquid density data of the 2-propanol (1) + water (2) mixture. (a) Training data: ◇, Stringari et al.;[8] □, Wagner and Pruβ;[9] ▲, this work. (b) Validation data: ⊕, Kubota et al.;[20] ■, Egorov et al.;[12] ○, Arce et al.;[15] ●, Boned et al.;[16] ▽, Origlia-Luster and Woolley;[14] ⊗, Friedman and Scheraga;[23] △, Hyncica et al.;[13] +, Sakurai;[19] ♦, Rauf et al.;[18] ⊖, Roux et al.;[22] ×, Schulte et al.;[17] *, Høiland;[21] ▼, Grigiante et al.[11]

A logistic function is assumed as the transfer function

$$g(z) = \frac{1}{1 + e^{-\beta \cdot z}} \tag{10}$$

W_1 represents the density, while V_i, for $i = 1$, 2, and 3, are temperature, pressure, and 2-propanol molar fraction x_1, respectively.

4.3. Bubble Pressure Model. Bubble pressure, P^{bub}, as a function of temperature and composition has been represented as

$$P^{\text{bub}}(T, x_1) = x_1 P_1^{\text{sat}} + (1 - x_1) P_2^{\text{sat}} + x_1(1 - x_1) \cdot W_1 \tag{11}$$

where P_1^{sat} and P_2^{sat} are the 2-propanol and water saturated pressure as a function of temperature calculated by the saturated pressure equations in ref 10 and in ref 9, respectively. In eq 11, W_1 is the denormalized output of a simple MLFN model in which V_i, for $i = 1$ and 2, are temperature and composition x_1, respectively. An arctangent function normalized in the range [0,1] is assumed as the transfer function

$$g(z) = \frac{1}{\pi} \arctan(\beta \cdot z) + 0.5 \tag{12}$$

5. Discussion

The measured values of liquid density and bubble pressure for the 2-propanol (1) + water (2) mixture have been represented by means of the models presented in section 4, and a statistical analysis of the data representation is reported herein.

In such a context, the error deviation Δ_i of the ith point, the percentage average absolute deviation AAD %, the bias %, and the percentage maximum absolute deviation MAD % with respect to a database of NPT values are evaluated as

$$\Delta_i = \left(\frac{M_{\text{exptl}} - M_{\text{calcd}}}{M_{\text{exptl}}} \right)_i \tag{13}$$

$$\text{AAD } \% = 100 \cdot \frac{1}{\text{NPT}} \sum_{i=1}^{\text{NPT}} |\Delta_i| \tag{14}$$

$$\text{bias } \% = 100 \cdot \frac{1}{\text{NPT}} \sum_{i=1}^{\text{NPT}} \Delta_i \tag{15}$$

$$\text{MAD } \% = 100 \cdot \max_{i=1,\text{NPT}} |\Delta_i| \quad (16)$$

where the generic property M represents the liquid density ρ or the bubble pressure p^{bub}.

The measured liquid density values, together with the liquid density values of pure 2-propanol[8] and of pure water,[9] at the same temperatures of the mixture measurements and for pressures ranging from the pure fluid bubble points up to 10 MPa, were used as training data to regress the parameters of a MLFN density model (eq 9). These parameters are presented in Table 2.

The obtained density model has been validated against literature data in the same range of temperatures and pressures.

Table 3 presents the accuracy of the density model with respect to the training data and the validation data. Figure 4 shows graphically the errors presented in Table 3. A very good representation is achieved for the 443 points used as training data (AAD % = 0.009; bias % = 0.004). The density model regressed on the training data represents the whole available density data (1137 points) in the considered range (x_1 = 0.00 to 1.00; T = (288 to 350) K; $P \leq$ 10.24 MPa) with an error (AAD % < 0.05) inside the experimental uncertainty of the density measurements.

Using the obtained density model, the excess molar volumes have been calculated, and their composition dependence has been shown in Figure 5a, varying pressure at constant temperature, and in Figure 5b, varying temperature at constant pressure. A very good agreement between experimental excess volume values and values predicted by the MLFN can be noted in Figure 5. This result comes from the very low residual error (AAD % = 0.009) in the representation of the pure fluids and of the measured mixture density values with the MLFN model. Figure 5 shows also a comparison with the excess volumes measured by Sakurai,[19] Egorov et al.,[12] and Boned et al.[16] A good agreement between the excess molar volumes predicted by the MLFN density model and the cited experimental data can be noted.

The coefficients of the MLFN involved in the bubble pressure model as a function of temperature and composition, eq 11, have been regressed on the literature bubble pressure values and on the saturated pressure of the pure 2-propanol[10] and pure water.[9] The parameters used for the correlation of the bubble

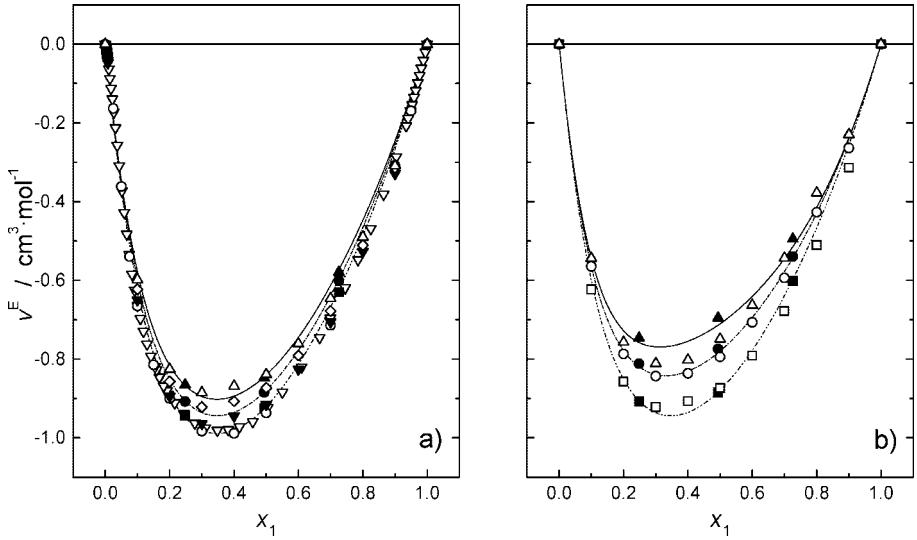

Figure 5. Excess molar volumes for the 2-propanol (1) + water (2) mixture. (a) Pressure dependence at constant temperature: ••–••–, MLFN, 0.1 MPa; •–•–•–, MLFN, 5.0 MPa; —, MLFN, 10.0 MPa; ■, this work, 0.1 MPa; ●, this work, 5.0 MPa; ▲, this work, 10.0 MPa; ▽, Sakurai,[19] 0.1 MPa; ○, Egorov et al.,[12] 0.1 MPa; ▼, Boned et al.,[16] 0.1 MPa; ◇, Boned et al.,[16] 5.0 MPa; △, Boned et al.,[16] 10.0 MPa. (b) Temperature dependence at constant pressure: ••–••–, MLFN, 300 K; •–•–•–, MLFN, 325 K; —, MLFN, 350 K; ■, this work, 300 K; ●, this work, 325 K; ▲, this work, 350 K; □, Boned et al.,[16] 303 K; ○, Boned et al.,[16] 323 K; △, Boned et al.,[16] 343 K.

Table 4. Parameters of the Feedforward Neural Network Involved in the Bubble Pressure Model, Equation 11, for the Mixture 2-Propanol (1) + Water (2)

$\beta = 0.5$			$V_{\text{min},1} = T_{\text{min}} = 260$			$V_{\text{max},1} = T_{\text{max}} = 400$		
$I = 3$			$V_{\text{min},2} = x_{\text{min}} = 0$			$V_{\text{max},2} = x_{\text{max}} = 1$		
$J = 8$			$W_{\text{min},1} = P^{\text{bub}}_{\text{min}} = 0$			$W_{\text{max},1} = P^{\text{bub}}_{\text{max}} = 10$		
$K = 1$								
i	j	w_{ij}	i	j	w_{ij}	j	k	w_{jk}
1	1	2.07887	2	5	2.49586	1	1	−2.73155
1	2	−9.89624	2	6	1.82237	2	1	−6.95864
1	3	−9.00570	2	7	7.67651	3	1	$-1.10463 \cdot 10^{1}$
1	4	7.02491	2	8	4.55245	4	1	3.38399
1	5	6.07017	3	1	$-8.25943 \cdot 10^{-1}$	5	1	5.52538
1	6	3.19986	3	2	4.18945	6	1	−3.98819
1	7	−4.60675	3	3	4.13969	7	1	5.93730
1	8	$-8.25220 \cdot 10^{-1}$	3	4	−2.98387	8	1	2.53652
2	1	1.67302	3	5	−6.41113	9	1	$-4.43300 \cdot 10^{-1}$
2	2	6.71506	3	6	−2.03992			
2	3	$1.71764 \cdot 10^{1}$	3	7	$7.19708 \cdot 10^{-1}$			
2	4	−1.40865	3	8	−2.38406			

Table 5. Accuracy of the Feedforward Neural Network Model, Equation 11, in the Representation of the Bubble Pressure Data of the 2-Propanol (1) + Water (2) Mixture

ref	NPT	*T* range (K)	*P* range (MPa)	x_1 range	AAD (%)	bias (%)	MAD (%)
Arce et al.[24]	27	353 to 372	0.10	0.00 to 0.98	0.914	−0.883	3.735
Khalfaoui et al.[25]	12	352 to 373	0.10	0.00 to 1.00	2.476	1.792	7.381
Marzal et al.[26]	78	325 to 373	0.03 to 0.10	0.00 to 1.00	1.494	0.465	6.231
Tsuji et al.[27]	10	298	0.01	0.07 to 0.90	0.554	0.177	2.571
Gironi and Lamberti[28]	32	353 to 373	0.10	0.00 to 1.00	1.229	0.041	6.102
Wu et al.[29]	21	353	0.05 to 0.10	0.00 to 1.00	0.844	−0.426	2.640
Sada and Morisue[30]	48	308 to 359	0.01 to 0.10	0.05 to 0.86	1.462	−1.031	3.017
Kato et al.[31]	17	353 to 370	0.10	0.01 to 1.00	1.646	−1.630	5.096
Ramalho and Drolet[32]	50	335 to 374	0.04 to 0.17	0.02 to 1.00	1.359	0.971	16.068
Wilson and Simmons[33]	99	309 to 373	0.01 to 0.10	0.00 to 1.00	0.974	−0.156	5.151
Brunjes and Bogart[34]	27	353 to 372	0.10	0.00 to 0.93	1.524	1.498	8.237
	421	298 to 374	0.01 to 0.17	0.00 to 1.00	1.276	0.058	16.068

Table 6. Saturated Liquid Densities for the 2-Propanol (1) + Water (2) Mixture

T/K	x_1	*P*/MPa	ρ/kg·m^{-3}
300.08	0.2483	0.0070	895.51
325.10	0.2483	0.0273	874.07
350.18	0.2483	0.0844	850.19
300.10	0.4939	0.0072	837.98
325.09	0.4939	0.0286	814.94
350.15	0.4939	0.0880	789.82
300.08	0.7258	0.0073	805.50
325.13	0.7258	0.0292	782.68
351.14	0.7258	0.0932	756.90

pressure data are presented in Table 4. The percentage errors of the bubble pressure model, eq 11, with respect to the bubble pressure data available from the literature in the temperature range from (298 to 374) K are presented in Table 5. The bubble pressure model represents the considered 421 points of the literature with AAD % < 1.3. The AAD % value is quite homogeneous for all the data sets involved in the regression of the MLFN coefficients, and the bias % value of 0.058 shows that the model is well centered with respect to the whole data set. A comparison between the bubble pressure model and the literature data presented in Table 5 is shown in Figure 6. In Figure 6a, the model of eq 11 has been compared with bubble temperature data. In such a figure, lines were obtained inverting eq 11 to calculate the bubble temperature as a function of pressure and composition. In Figure 6b, the model of eq 11 has been compared with bubble pressure data.

Saturated liquid density values can be obtained through the intersection of eq 9 for the compressed liquid density and eq 11 for the bubble pressure. In Table 6, the saturated liquid density values obtained with this procedure for the temperatures and compositions corresponding to the density measurements presented in this work are reported. Figure 7 shows the saturated liquid densities obtained with this procedure in the whole composition range and for temperatures from (287 to 350) K. The figure shows several isothermal sections pointing out the regular trends in the saturated liquid density representation by the developed model.

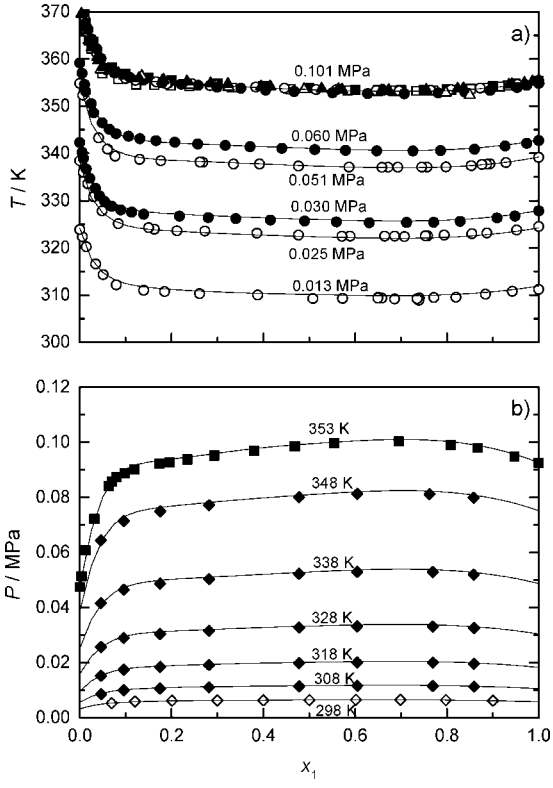

Figure 6. Representation of the bubble point model in comparison with the saturated data for the 2-propanol (1) + water (2) mixture: (a) bubble temperatures; (b) bubble pressures. □, Brunjes et Bogart;[34] ■, Wu et al.;[29] ○, Wilson and Simons;[33] ●, Marzal et al.;[26] △, Khalfaoui et al.;[25] ▲, Gironi and Lamberti;[28] ◇, Tsuji et al.;[27] ♦, Sada and Morisue;[30] —, bubble pressure model, eq 11.

6. Conclusions

Liquid densities for the 2-propanol (1) + water (2) mixture have been measured at (300, 325, and 350) K from 10 MPa down to about atmospheric pressure and x_1 molar fraction close to 0.25, 0.49, and 0.73. The measured liquid density values have been correlated with a MLFN including liquid density values of the pure components, showing a good consistency of the mixture measurements with the pure fluid data. The MLFN

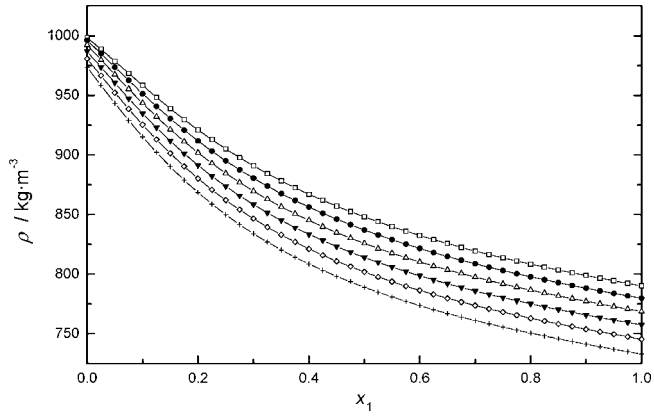

Figure 7. Saturated liquid density prediction for the 2-propanol (1) + water (2) mixture obtained as an intersection of the compressed liquid density model, eq 9, and the bubble pressure model, eq 11: –□–, 287.5 K; –●–, 300.0 K; –△–, 312.5 K; –▼–, 325.0 K; –◇–, 337.5 K; –+–, 350.0 K.

model was compared with the available literature data in the same range of temperatures and pressures showing a prediction accuracy of the same magnitude of the usually claimed experimental uncertainty for the experimental density measurements. Excess molar volumes have been calculated and compared with the excess volume measurements available from the literature in the same range.

A bubble pressure model combining a MLFN function and saturated pressure equations for the pure fluids was obtained correlating the literature bubble pressures for the 2-propanol (1) + water (2) mixture in the temperature range from (298 to 374) K.

The saturated liquid density surface in the temperature range of the measurements presented in this work has been obtained as an intersection of the compressed liquid density model and the bubble pressure model.

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