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Liquid Density Measurements for the Propylene + 2-Propanol + Water System

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Liquid densities for the propylene (1) + 2-propanol (2) + water (3) mixture have been determined at (300, 325, and 350) K from 10 MPa down to about the bubble pressures and for the molar fractions ($x_1 = 0.09$; $x_2 = 0.37$), ($x_1 = 0.18$; $x_2 = 0.38$), ($x_1 = 0.30$; $x_2 = 0.50$), ($x_1 = 0.39$; $x_2 = 0.42$), and ($x_1 = 0.61$; $x_2 = 0.30$) using a vibrating tube densimeter. The measured liquid density values have been correlated with a multilayer feedforward neural network (MLFN) function including liquid densities values of the propylene + 2-propanol mixture, of the 2-propanol + water mixture, and of the pure components in the temperature range from (300 to 350) K and in the pressure range up to 10 MPa. The consistency of the ternary mixture measurements with those of the binary mixtures and with pure fluids data is very good. The MLFN model shows an accuracy of the same magnitude of the claimed experimental uncertainty for the experimental density measurements.

Introduction

Many productions of the chemical industry present relevant energy consumption as in the case of the separation processes of fluid mixtures. For these processes, there is then a rising need to study new methods compatible with energy saving, environmental impact, and sustainable development. These goals could be achieved searching for separation processes alternative to the conventional ones.

The limited capabilities of the traditional modeling methods in representing the thermodynamics of complex systems, as for instance the ternary mixtures of polar and associating components, hinder the development of analysis and optimization studies for the production processes of such systems with respect to both the overall effectiveness and the energetic consumption.

Dealing with separation processes, the recovery of oxychemicals from aqueous solutions has received increasing attention, but the corresponding literature is still fragmented and incomplete for the cited purpose. To proceed efficiently, it is then necessary to start choosing a system on which to develop an exemplifying study. After a literature search, the 2-propanol dehydration, using propylene as solvent, appears to be a suitable system for this study. The system 2-propanol + water forms an azeotrope[1] preventing the 2-propanol separation through conventional distillation. On the other hand, 2-propanol has important industrial applications as a raw material in paint and ink products and as solvent in electronics and in medicine.

The propylene + 2-propanol + water system is thermodynamically strongly deviating from ideal behavior due to the strong polarity of the components, their association behavior, etc., which makes difficult a complete and accurate thermodynamic representation. Moreover, the literature is quite lacking in thermodynamic experimental data so that the foreseen study must start from an experimental activity.

The available experimental data includes phase equilibria by Zabaloy et al.[2] and Rojas et al.[3] for vapor−liquid equilibrium (VLE) and liquid−liquid equilibrium (LLE), respectively. Solubility data are also available from Wu et al.,[4] while VLLE data for the ternary mixture and H^E data for the same ternary and the binary 2-propanol + water system have been measured by Grigiante et al.[5]

For the density measurements, a "synthetic open circuit method", taking advantage of a vibrating tube densimeter (VTD), was used allowing one to obtain density data; this is one of the most popular measuring methods of the literature.

The compressed liquid density values, including liquid density values of the binary mixtures propylene + 2-propanol and 2-propanol + water and of the pure components, have been correlated by means of a multilayer feedforward neural network (MLFN) function.

This function has been also used to study the composition dependence of the excess volumes at constant temperature and pressure.

Experimental Section

Chemicals. The propylene (molar mass = 42.08 g·mol^{-1}, CAS Number 115-07-1) is from Air Liquide with a certified purity higher than 99.99 % in volume. The 2-propanol (molar mass = 60.096 g·mol^{-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. R134a (molar mass = 102.03 g·mol^{-1}, CAS Number 811-97-2) was purchased from Arkema (France) with a certified purity of 99.95 % in volume.

Apparatus and Experimental Procedure. A detailed description of the apparatus is given in ref 6, and its schematic layout is presented in ref 7. The apparatus employs synthetic mixtures that have been prepared gravimetrically under vacuum according to the procedures presented in ref 8. The forced path mechanical calibration (FPMC)[9] has been used for the calibration of the experimental apparatus.

Readers are encouraged to look for details about the experimental procedure in ref 7.

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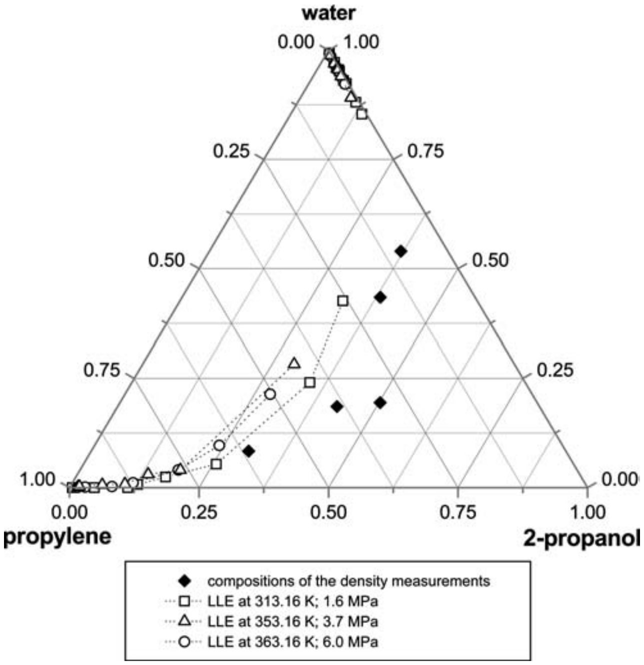

Figure 1. Compositions of the mixtures used for the experimental measurements and compositions of the LLE data from the literature.[3]

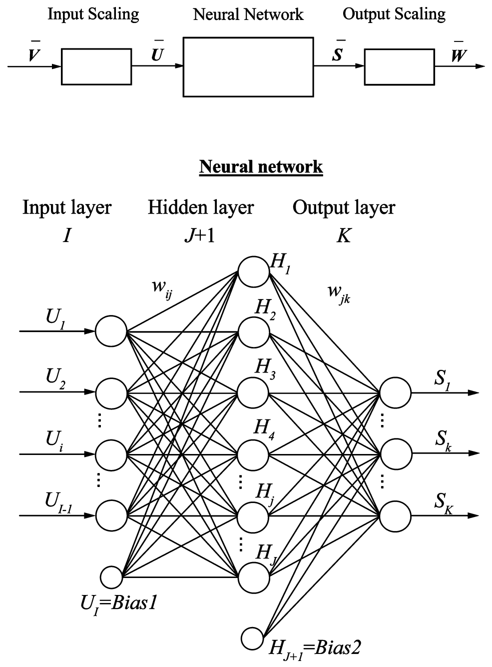

Figure 2. General topology of a three-layer feedforward neural network.

Experimental Uncertainties. The experimental uncertainties have been calculated taking into account the expanded uncertainties and coverage factor as described in ref 10. The combined expanded ($k = 2$) uncertainty on density data in the liquid phase is estimated to be 0.1 $\text{kg}\cdot\text{m}^{-3}$, therefore the corresponding relative uncertainty is within 0.05 %. For the calculation of the combined standard uncertainty of the density measurements the standard uncertainties of T, p, τ, and τ_0 have been taken into account, together with the accuracy of the equation-of-state (EoS) used to determine the density of the reference fluid. The state variables have been treated as independent of each other, so the covariance has been not considered. The uncertainty on vibrating period values is $\pm 10^{-8}$ s. The standard uncertainties on temperature measurements are estimated to be about ± 0.02 K and on pressure measurement are ± 0.0001 MPa (for $0 < p \le 0.6$ MPa) and ± 0.0006 MPa (for $0.6 < p \le 10.6$ MPa). Uncertainties in mixture composition are within $2\cdot10^{-4}$ in mole fraction.

Experimental Results

Liquid density values have been measured for the propylene (1) + 2-propanol (2) + water (3) mixture at about (300, 325, and 350) K from 10 MPa down to about the bubble pressures and for the following mole fractions: ($x_1 = 0.09$; $x_2 = 0.37$), ($x_1 = 0.18$; $x_2 = 0.38$), ($x_1 = 0.30$; $x_2 = 0.50$), ($x_1 = 0.39$; $x_2 = 0.42$), and ($x_1 = 0.61$; $x_2 = 0.30$). The measured (P, ρ, T, x) values are reported in Table 1. In Figure 1, the compositions of the mixtures used for the experimental measurements are reported on a ternary diagram where the available LLE data[3] are also reported showing that all the present measurements fall in the single phase liquid region.

Modeling Methods

General Features of the Multilayer Feedforward Neural Network. A multilayer feedforward neural network (MLFN) functional form has been used to correlate the experimental compressed liquid density values. The general architecture of a MLFN is illustrated in Figure 2; it is composed of a certain number of units, called neurons, organized in three layers named 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

$$U_I = Bias\ 1 \tag{1}$$

The number of neurons of the input 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

$$H_{J+1} = Bias\ 2 \tag{2}$$

The physical input variables V_i (temperature, pressure, and mole fractions for the components 1 and 2) undergo a linear transformation to normalize them in the arbitrarily chosen range [$A_{\min}$, $A_{\max}$] set as $A_{\min} = 0.05$ and $A_{\max} = 0.95$

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

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.

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

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

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

The symbols w_{ij} and w_{jk} indicate the weighting factors that are the free parameters of the model, which must be determined

Table 1. Experimental Liquid Density Data for the Propylene (1) + 2-Propanol (2) + Water (3) Mixture

p/MPa	ρ/(kg·m^{-3})	p/MPa	ρ/(kg·m^{-3})	p/MPa	ρ/(kg·m^{-3})	p/MPa	ρ/(kg·m^{-3})	p/MPa	ρ/(kg·m^{-3})	p/MPa	ρ/(kg·m^{-3})
$x_1 = 0.0904$; $x_2 = 0.3697$											
T = 305.05 K		T = 325.13 K		T = 350.16 K		T = 305.05 K		T = 325.13 K		T = 350.16 K	
0.4810	805.22	1.0965	787.78	1.9794	760.95	5.5576	809.63	6.1588	792.87	6.3886	767.42
0.7999	805.53	1.3765	788.08	2.2506	761.47	5.9644	809.96	6.5713	793.27	6.7535	767.93
1.1189	805.81	1.7884	788.50	2.6532	762.19	6.3666	810.30	6.9706	793.68	7.1751	768.45
1.5873	806.21	2.2055	788.92	2.7894	762.47	6.7866	810.64	7.3611	794.07	7.5340	768.95
1.9738	806.57	2.5256	789.26	3.1725	763.00	7.2071	810.99	7.7525	794.47	7.8862	769.36
2.3437	806.88	2.9169	789.68	3.4877	763.47	7.6091	811.32	8.1263	794.84	8.2903	769.86
2.8616	807.33	3.3853	790.18	3.8192	763.99	8.0286	811.65	8.5563	795.24	8.7023	770.37
3.0889	807.54	3.7252	790.51	4.1715	764.47	8.4590	812.01	8.9514	795.67	8.9884	770.84
3.6201	807.99	4.1353	790.90	4.5587	764.96	8.8724	812.34	9.3597	796.03	9.3719	771.35
3.9484	808.27	4.5483	791.31	4.9036	765.44	9.2723	812.66	9.7832	796.45	9.6929	771.80
4.3454	808.61	4.9428	791.70	5.2727	765.96	9.6791	812.99	10.1933	796.86	10.0187	772.34
4.7510	808.95	5.3524	792.10	5.6052	766.43	10.0684	813.35				
5.1507	809.29	5.8171	792.53	5.9927	766.93						
$x_1 = 0.1828$; $x_2 = 0.3828$											
T = 300.10 K		T = 325.11 K		T = 345.10 K		T = 300.10 K		T = 325.11 K		T = 345.10 K	
1.0199	758.54	1.8728	738.13	2.2984	718.81	5.8503	763.93	6.4030	743.98	5.9446	724.83
1.3355	758.91	2.2723	738.62	2.3475	718.97	6.3272	764.42	6.7761	744.45	6.1833	725.19
1.6925	759.33	2.5648	739.03	2.7307	719.58	6.6228	764.75	7.0992	744.86	6.4859	725.68
2.0684	759.75	2.8425	739.43	2.9939	720.06	6.9543	765.10	7.4957	745.33	6.7904	726.18
2.5068	760.25	3.1636	740.00	3.2842	720.53	7.4566	765.62	7.8402	745.77	7.0883	726.63
2.8233	760.61	3.4603	740.41	3.5454	720.93	7.8439	766.01	8.2173	746.22	7.3961	727.11
3.2665	761.10	3.8021	740.80	3.9537	721.63	8.2379	766.41	8.5721	746.68	7.6975	727.55
3.5650	761.44	4.2055	741.30	4.1125	721.93	8.6408	766.82	8.9346	747.14	8.0104	728.03
3.9100	761.82	4.5705	741.79	4.4260	722.46	9.0641	767.26	9.2711	747.56	8.3245	728.51
4.3613	762.31	4.9121	742.16	4.7064	722.89	9.4705	767.67	9.6208	747.98	8.6350	728.98
4.6798	762.67	5.3304	742.65	5.0009	723.31	9.8583	768.09	10.0454	748.47	8.9472	729.42
5.0641	763.09	5.7023	743.08	5.2821	723.84					9.2760	729.90
5.4541	763.51	6.0691	743.56	5.5902	724.30						
$x_1 = 0.3031$; $x_2 = 0.5024$											
T = 300.10 K		T = 325.13 K		T = 350.13 K		T = 300.10 K		T = 325.13 K		T = 350.13 K	
0.9309	707.92	1.1870	678.16	2.4368	653.52	5.9734	714.47	5.6730	685.61	6.4190	662.19
1.1970	708.29	1.4432	678.62	2.6048	653.96	6.4374	715.04	6.0311	686.15	6.7620	662.87
1.5561	708.78	1.7278	679.11	2.9301	654.68	6.8139	715.51	6.4017	686.72	7.0907	663.50
1.9481	709.29	2.1436	679.80	3.2025	655.27	7.2457	716.02	6.7892	687.28	7.4234	664.19
2.4588	709.93	2.4797	680.35	3.7344	656.44	7.6762	716.54	7.1736	687.86	7.7731	664.87
2.7801	710.37	2.8914	681.10	3.8724	656.79	8.0953	717.04	7.5690	688.43	8.1258	665.54
3.1645	710.88	3.1544	681.59	4.1369	657.40	8.5271	717.54	7.9652	689.02	8.4760	666.19
3.5128	711.35	3.5318	682.22	4.4889	658.17	9.0259	718.13	8.3550	689.57	8.8295	666.84
4.0090	711.99	3.8344	682.74	4.8105	658.86	9.4290	718.61	8.7637	690.16	9.1905	667.56
4.3604	712.44	4.1041	683.18	5.1260	659.50	9.7855	719.09	9.1707	690.73	9.5447	668.20
4.7663	712.95	4.5529	683.87	5.4452	660.17	10.2138	719.60	9.5748	691.28	9.9024	668.83
5.1546	713.45	4.9137	684.44	5.7662	660.85			9.9694	691.84		
5.5805	713.98	5.2916	685.03	6.0928	661.51						
$x_1 = 0.3906$; $x_2 = 0.4236$											
T = 300.10 K		T = 325.11 K		T = 350.11 K		T = 300.10 K		T = 325.11 K		T = 350.11 K	
1.0187	680.98	1.9518	650.66	2.6205	618.74	5.5919	687.54	6.2780	658.79	6.5680	629.17
1.1998	681.27	2.3561	651.45	3.0072	619.87	5.9575	688.05	6.6596	659.45	6.8828	629.92
1.6209	681.88	2.5960	651.95	3.1830	620.39	6.3307	688.56	7.0051	660.05	7.2018	630.66
1.9773	682.39	2.9341	652.61	3.5281	621.38	6.7084	689.06	7.3645	660.65	7.5611	631.49
2.3279	682.91	3.2077	653.19	3.7312	621.97	7.0811	689.56	7.7307	661.26	7.9087	632.29
2.7039	683.48	3.4938	653.75	4.0884	622.82	7.4649	690.07	8.1192	661.90	8.2357	633.07
3.0296	683.95	3.8787	654.46	4.3645	623.63	7.8655	690.59	8.4743	662.48	8.5847	633.86
3.3633	684.43	4.2234	655.08	4.6536	624.39	8.2519	691.10	8.8572	663.10	8.9126	634.62
3.7581	685.00	4.5679	655.73	4.9512	625.19	8.6313	691.60	9.2336	663.72	9.2911	635.35
4.0323	685.37	4.8926	656.32	5.2582	625.98	9.0140	692.09	9.6192	664.33	9.6659	636.22
4.4872	686.01	5.2235	656.91	5.5968	626.78	9.4229	692.60	9.9714	664.93	9.9874	636.95
4.8414	686.51	5.5586	657.52	5.9458	627.64	9.8324	693.12				
5.2112	687.02	5.9273	658.17	6.2382	628.34						
$x_1 = 0.6123$; $x_2 = 0.3039$											
T = 300.10 K		T = 325.12 K		T = 350.10 K		T = 300.10 K		T = 325.12 K		T = 350.10 K	
1.0854	614.94	1.8941	580.11	2.8501	540.02	5.4945	623.39	5.5629	590.47	6.0943	553.32
1.5314	615.81	2.2073	580.96	3.0168	540.87	5.8751	624.07	5.9303	591.32	6.4191	554.43
1.8707	616.53	2.5281	581.84	3.2315	541.94	6.2521	624.73	6.3212	592.20	6.7321	555.54
2.3726	617.48	2.8474	582.67	3.5057	543.11	6.6365	625.40	6.6863	593.02	7.0480	556.69
2.5272	617.84	3.2008	583.61	3.7827	544.27	7.0329	626.07	7.0575	593.82	7.3729	557.82
2.9221	618.61	3.4991	584.39	3.9965	545.27	7.4534	626.76	7.4688	594.69	7.7030	558.93
3.2262	619.19	3.7780	585.12	4.3281	546.57	7.8662	627.47	7.8762	595.54	8.0598	559.96
3.5794	619.86	3.8175	586.14	4.6211	547.80	8.2557	628.11	8.2536	596.34	8.4385	561.12
4.0682	620.74	4.2142	587.19	4.8667	548.79	8.6619	628.75	8.6532	597.15	8.8208	562.37
4.2817	621.17	4.5221	587.93	5.1693	550.07	9.0796	629.46	9.0784	597.99	9.1877	563.44
4.7290	622.00	4.8663	588.81	5.4573	551.09	9.4742	630.08	9.5001	598.83	9.5755	564.54
5.1095	622.68	5.2102	589.63	5.7592	552.24	9.8967	630.79	9.9155	599.65	9.9391	565.57

Table 2. Parameters of the Feedforward Neural Network Used for the Correlation of the Liquid Density Data for the Propylene (1) + 2-Propanol (2) + Water (3) Mixture

$\beta = 0.5$, $I = 5$, $J = 12$, $K = 1$			$V_{\min,1} = T_{\min} = 250$, $V_{\min,2} = P_{\min} = 0$, $V_{\min,3} = x_{1,\min} = 0$, $V_{\min,4} = x_{2,\min} = 0$, $W_{\min,1} = \rho_{\min} = 250$			$V_{\max,1} = T_{\max} = 400$, $V_{\max,2} = P_{\max} = 12$, $V_{\max,3} = x_{1,\max} = 1$, $V_{\max,4} = x_{2,\max} = 1$, $W_{\max,1} = \rho_{\max} = 1050$					
i	j	w_{ij}	i	j	w_{ij}	i	j	w_{ij}	j	k	w_{jk}
1	1	$-2.92762 \cdot 10^{1}$	3	1	$-1.99930 \cdot 10^{1}$	5	1	$-1.75403 \cdot 10^{1}$	1	1	$4.58186 \cdot 10^{1}$
1	2	4.21347	3	2	−6.66933	5	2	$5.40361 \cdot 10^{-3}$	2	1	$-3.38637 \cdot 10^{1}$
1	3	2.47330	3	3	−1.49965	5	3	−1.24796	3	1	$2.68326 \cdot 10^{1}$
1	4	−4.47885	3	4	−3.35238	5	4	$-1.27458 \cdot 10^{-1}$	4	1	1.27324
1	5	2.72143	3	5	$-6.83433 \cdot 10^{-1}$	5	5	−1.53151	5	1	$-2.25387 \cdot 10^{1}$
1	6	−5.43393	3	6	1.71319	5	6	$1.24410 \cdot 10^{1}$	6	1	$-1.75728 \cdot 10^{1}$
1	7	3.52922	3	7	$3.09508 \cdot 10^{1}$	5	7	−3.00794	7	1	$-2.98598 \cdot 10^{1}$
1	8	$-2.15646 \cdot 10^{1}$	3	8	$-1.71309 \cdot 10^{1}$	5	8	$2.86986 \cdot 10^{1}$	8	1	$-2.39993 \cdot 10^{1}$
1	9	4.42482	3	9	−7.10556	5	9	$7.95524 \cdot 10^{-2}$	9	1	$3.02683 \cdot 10^{1}$
1	10	$-2.08228 \cdot 10^{1}$	3	10	$-1.78988 \cdot 10^{1}$	5	10	$2.93360 \cdot 10^{1}$	10	1	$2.75980 \cdot 10^{1}$
1	11	$-1.61511 \cdot 10^{2}$	3	11	$-5.20945 \cdot 10^{1}$	5	11	$1.30889 \cdot 10^{2}$	11	1	6.70185
1	12	5.47497	3	12	$1.55951 \cdot 10^{1}$	5	12	−2.90082	12	1	$1.95301 \cdot 10^{1}$
2	1	1.88455	4	1	$-1.43946 \cdot 10^{1}$				13	1	$1.61961 \cdot 10^{1}$
2	2	$-1.88623 \cdot 10^{-1}$	4	2	−2.33862						
2	3	$-2.37482 \cdot 10^{-1}$	4	3	−2.14679						
2	4	$2.08989 \cdot 10^{-1}$	4	4	2.63885						
2	5	$-2.83151 \cdot 10^{-1}$	4	5	−2.55880						
2	6	2.97414	4	6	$3.26107 \cdot 10^{1}$						
2	7	$-5.42178 \cdot 10^{-2}$	4	7	$2.03028 \cdot 10^{1}$						
2	8	$1.10477 \cdot 10^{1}$	4	8	−1.37383						
2	9	$-1.82864 \cdot 10^{-1}$	4	9	−2.46377						
2	10	9.85172	4	10	−2.11137						
2	11	$9.06796 \cdot 10^{1}$	4	11	$4.02489 \cdot 10^{1}$						
2	12	$5.21938 \cdot 10^{-2}$	4	12	$2.33143 \cdot 10^{1}$						

in 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

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

where

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

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

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

$$\rho(T, P, x_1, x_2) = W_1 \tag{9}$$

An arctangent function normalized in the [0, 1] range is assumed as the transfer function

$$g(z) = \frac{1}{\pi}\arctan(\beta \cdot z) + 0.5 \tag{10}$$

where z is the argument of eqs 5 and 6. In it, V_i for $i = 1, 2, 3, 4$, as formerly exposed, is temperature, pressure, propylene mole fraction x_1, and 2-propanol mole fraction x_2, respectively.

Discussion

The measured values of liquid density for the propylene (1) + 2-propanol (2) + water (3) mixture have been represented by means of the model, eq 9, presented in the previous section and a statistical analysis of the data representation is reported in the following.

In such a context, the error deviation Δ_i of the i^{th} point, the average absolute deviation AAD %, the Bias %, and the percentage maximum absolute deviation MAD % with respect to a database of NPT values are evaluated as

$$\Delta_i = \left(\frac{\rho_{\text{exp}} - \rho_{\text{calc}}}{\rho_{\text{exp}}}\right)_i \tag{11}$$

$$\text{AAD\%} = 100 \cdot \frac{1}{\text{NPT}} \sum_{i=1}^{\text{NPT}} |\Delta_i| \tag{12}$$

$$\text{Bias\%} = 100 \cdot \frac{1}{\text{NPT}} \sum_{i=1}^{\text{NPT}} \Delta_i \tag{13}$$

$$\text{MAD\%} = 100 \cdot \max_{i=1,\text{NPT}} |\Delta_i| \tag{14}$$

The measured liquid density values for the propylene + 2-propanol + water mixture, together with the liquid density values for the propylene + 2-propanol mixture from ref 7 and for the 2-propanol + water mixture from ref 11, and liquid density values generated for the pure fluids propylene, 2-propanol, and water in the same range of temperature and pressure were correlated with the MLFN model presented in the former section. The MLFN parameters are presented in Table 2.

Table 3 presents the accuracy of the density model with respect to the training data for the systems propylene + 2-propanol + water, propylene + 2-propanol, 2-propanol + water, and for the pure components. For the propylene and water as pure components, the values generated from the dedicated equations-of-state in refs 12 and 13, respectively, have been used in the regression procedure; for 2-propanol, values generated through the Starling BWR equation developed in ref 14 have been used. Figure 3 shows graphically the errors presented in Table 3. A very good representation is achieved for the 1105 points used as training data (AAD = 0.035 %; Bias = 0.001 %); the density model represents the data with an error inside the experimental uncertainty of the density measurements. A better representation is achieved for the pure components in particular for 2-propanol (AAD = 0.009 %; Bias = 0.004 %)

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

system	ref	NPT[a]	*T* range (K)	*P* range (MPa)	x_1 range	x_2 range	AAD (%)	Bias (%)	MAD (%)
propylene (1) + 2-propanol (2) + water (3)	this work	378	300−350	0.47−10.21	0.09−0.61	0.30−0.50	0.052	−0.005	0.184
propylene (1) + 2-propanol (2)	Stringari et al.[7]	186	300−350	0.52−9.99	0.20−0.65	0.35−0.80	0.038	0.020	0.122
2-propanol (1) + water (2)	Stringari et al.[11]	200	300−351	0.07−10.24	0.00	0.25−0.73	0.035	−0.004	0.104
propylene	Angus et al.[12]	98	300−350	1.21−10.10	1.00	0.00	0.025	0.004	0.173
2-propanol	Stringari et al.[14]	123	300−350	0.01−10.00	0.00	1.00	0.009	0.004	0.026
water	Wagner et al.[13]	120	300−350	0.00−9.75	0.00	0.00	0.013	−0.002	0.036
		1105	300−351	0.00−10.24	0.00−1.00	0.00−1.00	0.035	0.001	0.184

[a] NPT: number of experimental points.

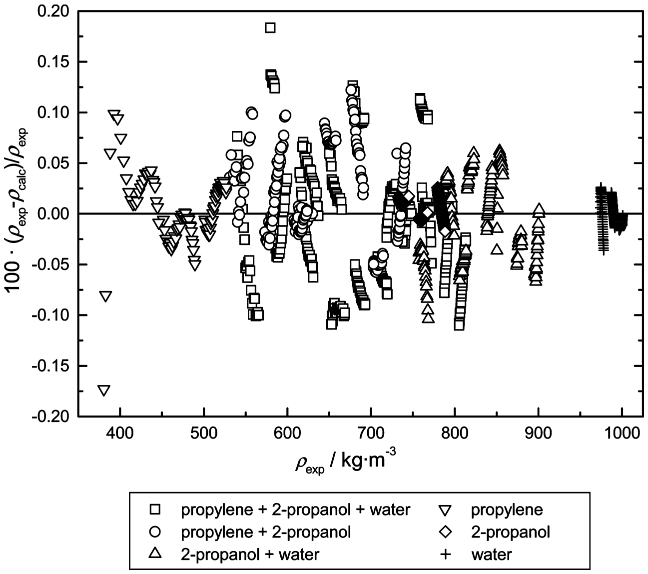

Figure 3. Percentage error of the feedforward neural network model, eq 9, in the representation of the liquid density data of the propylene + 2-propanol + water system.

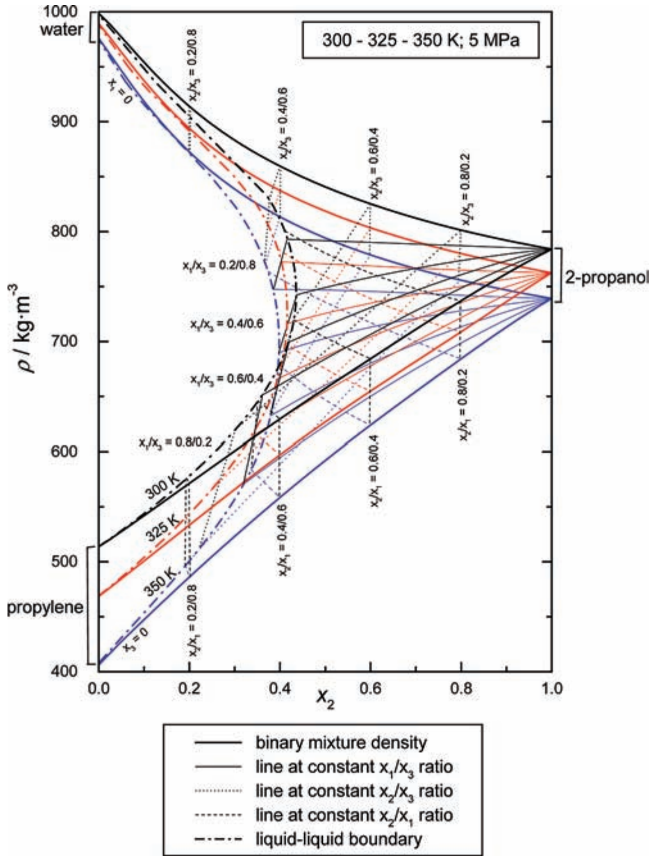

Figure 4. Liquid density surfaces for the propylene (1) + 2-propanol (2) + water (3) system obtained through the MLFN model, eq 9, for the temperatures (300, 325, and 350) K and for the constant pressure of 5 MPa.

and water (AAD = 0.013 %; Bias = −0.002 %), while a slight worsening is shown for propylene (AAD = 0.025 %; Bias = 0.004 %). The reason for this behavior is that the density surface in the considered range is very smooth for 2-propanol and water, while a greater curvature of the density surface exists for propylene due to the closeness of the considered range to the critical point of that fluid (T_c = 365.57 K, P_c = 4.665 MPa). The performance of the model for the two binary mixtures is very homogeneous with AAD less than 0.04 %. A slightly worse behavior is shown for the present ternary mixture measurements with respect to the ones of the cited binaries, presenting AAD of about 0.05 %, which is comparable with the claimed uncertainty of the experimental measurements. The Bias for the ternary mixture is −0.005 %. The MAD values show a low scattering for all of the data used to regress the model.

In Figure 4, the liquid density surfaces produced through the obtained MLFN model at (300, 325, and 350) K are shown at the constant pressure of 5 MPa. The propylene (1) + 2-propanol (2) + water (3) system has been represented in the whole composition range. The liquid−liquid boundaries at each temperature (see dash-dotted lines in the figure) have been obtained through a phase equilibrium G^E − EoS model for the propylene + 2-propanol + water system formerly presented in ref 5. The model has been composed by a Peng−Robinson cubic EoS with Wong−Sandler mixing rules and a modified UNIQUAC to represent the G^E function. The model has been regressed on phase equilibria and excess enthalpy data as discussed in detail in ref 5. Figure 4 shows the regular trends in the liquid density representation obtained by the developed model, eq 9.

In Figure 5, the excess molar volume surface of the propylene (1) + 2-propanol (2) + water (3) system, as represented by the density model, eq 9, is shown at 325 K and 5 MPa as a function of compositions. In this case too, the liquid boundary, represented by the aforementioned G^E − EoS model, is plotted with the dash-dotted line while constant composition lines are also drawn. The figure evidences the large volume deviation from ideality of the system of interest that confirms the difficulty in representing with high accuracy the whole thermodynamics of such a mixture, which is the goal of our present research program. On the other hand, the high effectiveness of the adopted MLFN method allows one to obtain a very precise representation of the volumetric properties, as it arises from Table 3 and Figures 3 to 5.

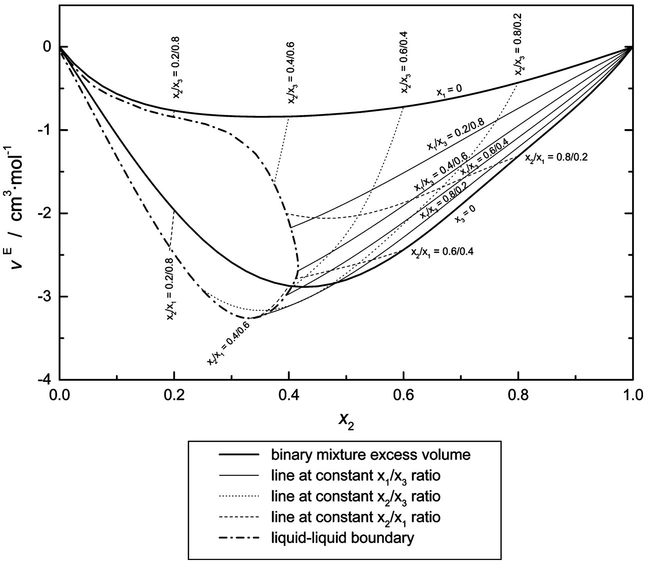

Figure 5. Excess volume surface for the propylene (1) + 2-propanol (2) + water (3) system obtained through the MLFN model, eq 9, at 325 K and 5 MPa.

Conclusions

The propylene (1) + 2-propanol (2) + water (3) system considered for the study of the extraction process of 2-propanol from the aqueous solution is of particular interest with respect to the thermodynamic point of view due to the strong polarity and associating behavior of the mixture components.

In the present work, the volumetric properties of the mixture have been investigated using a vibrating tube densimeter. Liquid densities for the propylene (1) + 2-propanol (2) + water (3) mixture have been measured at (300, 325 and 350) K from 10 MPa down to about the bubble pressures and for the following mole fractions: ($x_1 = 0.09$; $x_2 = 0.37$), ($x_1 = 0.18$; $x_2 = 0.38$), ($x_1 = 0.30$; $x_2 = 0.50$), ($x_1 = 0.39$; $x_2 = 0.42$), and ($x_1 = 0.61$; $x_2 = 0.30$). The global relative uncertainty on liquid density data is estimated to be within 0.05 %.

The effectiveness of the MLFN function in representing the volumetric properties has been exploited correlating both the measured liquid densities values including in the regression procedure also the liquid densities values of the propylene + 2-propanol mixture, of the 2-propanol + water mixture, and of the pure components, in the temperature range from (300 to 350) K and in the pressure range up to 10 MPa. The MLFN model represents the density values of the system of interest in the whole composition range with an individual accuracy of the same magnitude of the claimed experimental uncertainty for the experimental density measurements. Furthermore, a very good consistency of the ternary mixture measurements with those of the binary mixtures and with the values generated for the pure fluids have been demonstrated.

The liquid density surfaces at (300, 325, and 350) K and the excess molar volume surface at 325 K have been calculated in the whole composition range at the constant pressure of 5 MPa through the regressed MLFN model. The regular and smoothed trend of the surfaces points out the consistency among all the considered density values and the high effectiveness of the MLFN method for the representation of volumetric properties.

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