Experimental and Modeling of Densities and Viscosities of Binary Mixtures Containing MTBE/Alkan-2-ol

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The density and viscosity of three binary mixtures composed of methyl tert-butyl ether (MTBE) with 2-propanol, 2-butanol, and 2-pentanol over the whole composition range at 293.15-323.15 K were measured. The excess molar volume V_m^E and deviation in viscosity $\Delta\eta$, were calculated and interpreted in terms of intermolecular interactions among the species in the mixtures. For all binary mixtures, negative values of V_m^E and $\Delta\eta$ were fitted to the Redlich-Kister polynomial function. By increasing temperature, V_m^E and $\Delta\eta$ were reduced and increased, respectively. The density of the binary systems was modeled in terms of the perturbed chain statistical associating fluid theory (PC-SAFT) and compared with the corresponding experimental data. Maximum of deviation between the experimental data and calculated values by this theory is 1.4% and belongs to the MTBE + 2-butanol system.

INTRODUCTION

The physical properties of binary mixtures derived from densities and viscosities are important to study the type and extent of molecular interactions providing useful information on the molecular interactions. These properties such as thermal expansion coefficients or fluidity of mixtures are useful for many types of transport processes in chemical industries. Methyl tert-butyl ether (MTBE) is a volatile, flammable, and colorless liquid used to dissolve gallstones. This material has low pollutant and widely used as an octane booster for lead-free or low-leaded gasoline. Addition of MTBE cuts down exhaust emissions particularly carbon monoxide, unburned hydrocarbons, polycyclic aromatics, and particulate carbon [1].

A literature survey indicates that some studies were performed on thermophysical properties of MTBE and 2-alkanol systems. Also, some reports are available for thermodynamic properties such as excess molar enthalpy,

excess molar volumes, activity coefficients, and vapor liquid equilibria [2-5] for MTBE and 1-alkanol. Values of densities and viscosities of MTBE with 2-propanol along with the excess molar volumes and viscosity deviations at various temperatures are reported in ref. [6]. In addition, the densities and experimental data of vapor-liquid equilibria for MTBE + 2-propanol at different temperatures and pressures are available in ref. [7]. For binary mixtures of MTBE + 2-butanol, values of densities and viscosities at $T = 298.15$ K are presented in ref. [8]. In this paper, as a continuation of our work [9,10], we report an extended study on the thermophysical properties of binary mixtures containing MTBE + 2-propanol, 2-butanol, and 2-pentanol while trying to correlate the densities by the PC-SAFT model. Outcomes of this model are compared to the experimental data and deviations are reported based on the standard deviation.

EXPERIMENTAL

The chemicals (MTBE, 2-propanol, 2-butanol, and

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2-pentanol) used were of analytical grade and provided from Merck with the stated level of purity greater than 99%. Density and viscosity were measured with an automated SVM 3000 Anton-Paar Stabinger viscometer that operates based on the modified Couette principle with a rapidly rotating outer tube and an inner measuring bob which rotates more slowly. The relative uncertainty is 1×10^{-3} g cm^{-3} for density and 0.02 for viscosity measurements. Both density and viscosity are highly sensitive to temperature, so they were controlled by a built-in thermoelectric thermostat. Before each series of measurements, the apparatus was calibrated using doubly distilled degassed water and dry air at the atmospheric pressure. For measuring the density and viscosity, mixtures were prepared just before use, and all properties were simultaneously measured. The liquid mixtures were prepared by mass on an analytical balance (Mettler AE 163, Switzerland) with the precision of ±0. 01 mg. Cautions were taken to prevent evaporation of the samples after preparation. A set of ten compositions was prepared for each mixture, and their physical properties were measured in the mole fraction range. The estimated uncertainty in the mole fraction was $\pm 1 \times 10^{-4}$.

RESULTS AND DISCUSSION

Values of density and viscosity for pure compounds and binary mixtures at various temperatures are reported in Table 1. The excess molar volume, V_m^E was calculated using

$$V_m^E = \sum_{i=1}^{N} x_i M_i (\rho^{-1} - \rho_i^{-1})$$ (1)

where x_i is the mole fraction, M_i is the molar mass of component i, ρ is the density of the mixture, ρ_i is the density of pure component i, and N stands for the number of components in the mixture. V_m^E for the binary mixtures was fitted by the Redlich-Kister equation[11]:

$$V_m^E = x_1(1-x_1) \sum_{k=0}^{N} A_k (1-2x_1)^k$$ (2)

where x_1 is the mole fraction of MTBE and A_k is an adjustable coefficient. Values of V_m^E and viscosity deviation

aare reported in SI file, Table S1. The standard deviation was calculated using

$$\sigma = \left[\sum (V_{exp}^E - V_{cal}^E)^2 / (n-p) \right]^{1/2}$$ (3)

where V_{exp}^E and V_{cal}^E are the experimental and calculated data, respectively. Values of A_k and standard deviation are presented in SI file, Table S2.

Figure 1 illustrates the graphs of excess molar volumes of MTBE + 2-alkanol mixtures at $T = 298.15$ K. As the figure indicates, the excess molar volume of the system MTBE + 2-alkanol is negative. This behavior is expected for specific interactions between the functional groups of aliphatic ether and the polar alcohols. For the mentioned mixtures, the geometrical fitting of the ether into the alcohol structure and specific interactions among the unlike molecules are dominated factors on positive contributions caused by the disruption of associated alcohol structure. So, the attractive interactions are stronger in the MTBE + 2-alkanol systems. In the aforementioned mixtures, V_m^E increases in the following order: 2-propanol < 2-butanol < 2-pentanol. This trend indicates a more organized packing effect and stronger interactions in the shorter length alcohols, especially for MTBE + 2-propanol. Molecules of 2-propanol are less sterically hindered than 2-butanol or 2-pentanol leading to the strained structure and increases the availability of OH group to interact with ether.

The chemical interactions are getting weaker with increasing in the alkyl chain length of 2-alkanol. Formation of the structures with less ordering due to the rise of temperature decreases the interactions in the liquid mixtures and increases the excess molar volume. Similar behavior [6-8] was reported for the binary mixtures MTBE + 2-propanol, and 2-butanol. Values of V_m^E for the mentioned systems are negative and increase with increasing temperature. The negative V_m^E values are mainly attributed to the formation of H-bonds in the mixtures and fitting the molecules one component into the void space of other molecules. Maximum deviation between our data for binary mixtures MTBE + 2-propanol and values reported in ref. [6] is 4.8% for excess molar volumes and 3.76% for viscosity deviations. Also, the comparison between our excess molar volumes of MTBE + 2-propanol and values reported in ref.

Table 1. Densities ρ and Viscosities η for the Binary Mixtures at Various Temperatures

Methyl tert-butyl ether + 2-propanol							
ρ (g cm^{-3})							
x_1	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	318.15 K	323.15 K
0	0.7854	0.7811	0.7768	0.7724	0.7680	0.7634	0.7588
0.0811	0.7817	0.7771	0.7726	0.7680	0.7634	0.7586	0.7540
0.1598	0.7780	0.7734	0.7687	0.7639	0.7591	0.7543	0.7495
0.2396	0.7744	0.7696	0.7648	0.7598	0.7549	0.7500	0.7452
0.3497	0.7694	0.7644	0.7595	0.7544	0.7494	0.7443	0.7394
0.4397	0.7654	0.7603	0.7553	0.7502	0.7450	0.7399	0.7349
0.5596	0.7599	0.7548	0.7497	0.7445	0.7392	0.7340	0.7291
0.6497	0.7560	0.7507	0.7456	0.7403	0.7350	0.7298	0.7248
0.7397	0.7520	0.7467	0.7415	0.7362	0.7309	0.7256	0.7207
0.8497	0.7472	0.7419	0.7367	0.7314	0.7260	0.7207	0.7153
0.9400	0.7433	0.7380	0.7328	0.7275	0.7220	0.7163	0.7106
1	0.7407	0.7354	0.7302	0.7247	0.7193	0.7133	0.7074
η (mPa s)							
0	2.42	2.08	1.80	1.56	1.36	1.19	1.05
0.0811	1.747	1.534	1.35	1.219	1.056	0.934	0.824
0.1598	1.318	1.177	1.047	0.967	0.832	0.727	0.648
0.2396	1.037	0.937	0.844	0.77	0.664	0.578	0.515
0.3497	0.791	0.722	0.665	0.595	0.52	0.44	0.368
0.4397	0.662	0.608	0.556	0.492	0.419	0.346	0.273
0.5596	0.539	0.500	0.452	0.392	0.328	0.26	0.191
0.6497	0.475	0.437	0.393	0.339	0.282	0.223	0.16
0.7397	0.421	0.385	0.353	0.312	0.26	0.21	0.15
0.8497	0.372	0.340	0.313	0.285	0.24	0.20	0.16
0.9400	0.353	0.331	0.301	0.275	0.24	0.209	0.178
1	0.345	0.32	0.297	0.275	0.252	0.231	0.206

Table 1. Continued

	Methyl tert-butyl ether + 2-butanol						
	ρ (g cm^{-3})						
x_1	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	318.15 K	323.15 K
0	0.8067	0.8027	0.7984	0.7941	0.7898	0.7852	0.7806
0.0810	0.8011	0.7969	0.7924	0.7879	0.7834	0.7786	0.7739
0.1600	0.7957	0.7913	0.7867	0.7820	0.7774	0.7725	0.7678
0.2400	0.7903	0.7857	0.7810	0.7762	0.7715	0.7665	0.7617
0.3500	0.7828	0.7781	0.7733	0.7684	0.7634	0.7584	0.7536
0.4400	0.7768	0.7720	0.7671	0.7621	0.7570	0.7520	0.7471
0.5600	0.7689	0.7639	0.7588	0.7538	0.7486	0.7434	0.7385
0.6500	0.7630	0.7579	0.7528	0.7477	0.7424	0.7372	0.7323
0.7401	0.7572	0.7520	0.7468	0.7416	0.7363	0.7311	0.7262
0.8500	0.7502	0.7449	0.7397	0.7344	0.7290	0.7238	0.7181
0.9398	0.7445	0.7392	0.7339	0.7287	0.7233	0.7175	0.7118
1	0.7407	0.7354	0.7302	0.7247	0.7193	0.7133	0.7074
	η (mPa s)						
0	3.67	3.04	2.54	2.13	1.80	1.54	1.33
0.0810	2.793	2.32	1.938	1.645	1.426	1.25	1.106
0.1600	2.063	1.76	1.468	1.233	1.054	0.92	0.819
0.2400	1.590	1.35	1.069	0.90	0.751	0.641	0.539
0.3500	1.210	1.01	0.771	0.586	0.463	0.354	0.245
0.4400	1.00	0.80	0.60	0.429	0.30	0.20	0.108
0.5600	0.810	0.613	0.457	0.313	0.20	0.10	0.046
0.6500	0.680	0.506	0.374	0.265	0.162	0.08	0.033
0.7401	0.580	0.443	0.333	0.245	0.156	0.10	0.053
0.8500	0.477	0.38	0.30	0.238	0.183	0.128	0.10
0.9398	0.400	0.35	0.292	0.251	0.217	0.19	0.162
1	0.345	0.32	0.297	0.275	0.252	0.231	0.206

Table 1. Continued

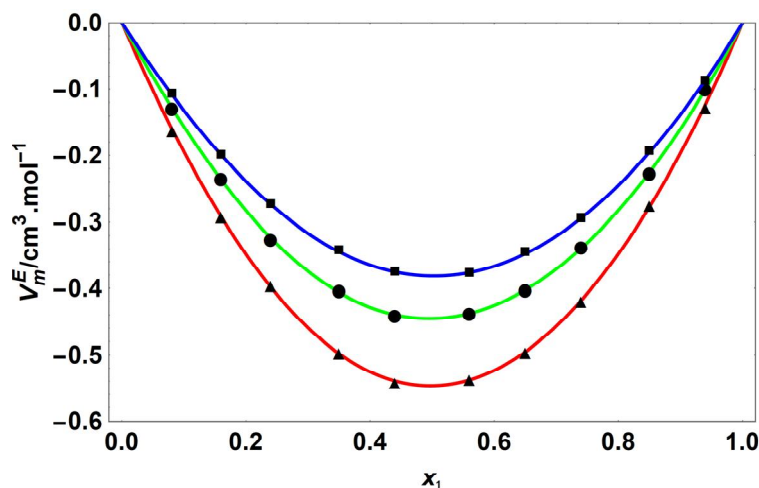|				Methyl tert-butyl ether + 2-pentanol			
				ρ (g cm^{-3})			
x_1	293.15 K	298.15 K	303.15 K	308.15 K	313.15 K	318.15 K	323.15 K
0	0.8093	0.8053	0.8012	0.7970	0.7927	0.7884	0.7840
0.0811	0.8041	0.7996	0.7953	0.7910	0.7865	0.7821	0.7776
0.1599	0.7990	0.7941	0.7897	0.7852	0.7806	0.7760	0.7714
0.2400	0.7938	0.7885	0.7840	0.7793	0.7746	0.7699	0.7652
0.3501	0.7864	0.7808	0.7761	0.7713	0.7664	0.7616	0.7568
0.4400	0.7803	0.7745	0.7697	0.7648	0.7598	0.7549	0.7501
0.5600	0.7720	0.7661	0.7612	0.7561	0.751	0.7460	0.7411
0.6500	0.7657	0.7598	0.7548	0.7497	0.7444	0.7394	0.7345
0.7400	0.7594	0.7535	0.7484	0.7432	0.7379	0.7328	0.7279
0.8499	0.7515	0.7458	0.7406	0.7354	0.7301	0.7249	0.7199
0.9400	0.7451	0.7396	0.7344	0.7291	0.7237	0.7179	0.7126
1	0.7407	0.7354	0.7302	0.7247	0.7193	0.7133	0.7074
				η (mPa s)			
0	3.97	3.32	2.81	2.37	1.99	1.66	1.39
0.0811	2.815	2.359	1.994	1.682	1.419	1.208	1.032
0.1599	1.943	1.633	1.378	1.181	1.001	0.849	0.744
0.2400	1.344	1.134	0.98	0.868	0.728	0.613	0.524
0.3501	0.97	0.823	0.705	0.617	0.514	0.412	0.345
0.4400	0.774	0.666	0.574	0.493	0.407	0.326	0.268
0.5600	0.621	0.546	0.474	0.407	0.337	0.275	0.226
0.6500	0.546	0.488	0.424	0.37	0.313	0.255	0.211
0.7400	0.496	0.441	0.39	0.341	0.296	0.243	0.200
0.8499	0.436	0.39	0.35	0.313	0.275	0.234	0.197
0.9400	0.39	0.355	0.321	0.292	0.263	0.231	0.200
1	0.345	0.32	0.297	0.275	0.252	0.231	0.206

Fig. 1. Excess molar volumes V_m^E *vs*. mole fraction of methyl tert-butyl ether for binary mixtures of methyl tert-butyl ether with (▲) 2-propanol, (●) 2-butanol, (■) 2-pentanol at $T = 298.15$ K. (——) Redlich-Kister equation.
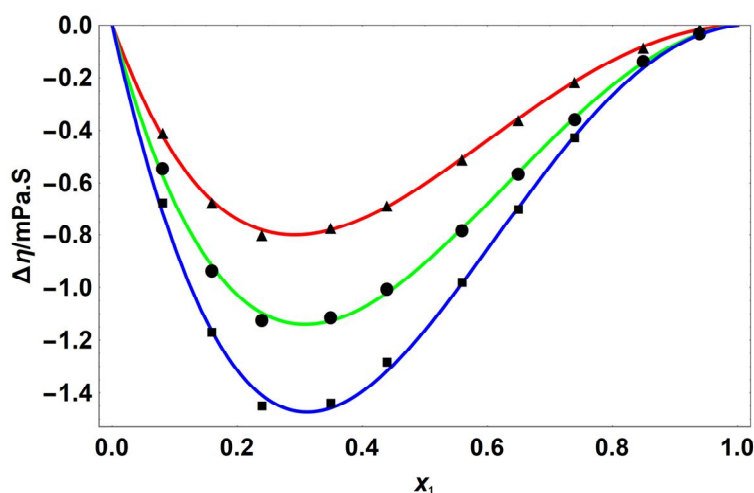

Fig. 2. Viscosity deviations $\Delta\eta$ *vs*. mole fraction of methyl tert-butyl ether for binary mixtures of methyl tert-butyl ether with (▲) 2-propanol, (●) 2-butanol, (■) 2-pentanol at $T = 298.15$ K. (——) Redlich-Kister equation.

[7] shows 3.67% deviation. The differences are due to various sources of materials (Merck, Fluka, Sigma, and so forth), amount and sort of impurity, and different techniques of measurement. Comparisons are reported in SI file. Also in refs. [12,13] values of excess molar enthalpy for binary systems MTBE + 2-propanol and 2-butanol are reported.

Data are positive (maximum value for MTBE + 2-propanol is 688 J mol^{-1} at mole fraction $x = 0.35$ and $T = 298.15$ K, and for binary mixture MTBE + 2-butanol is 947 J mol^{-1} at $x = 0.28$ and $T = 308.15$ K). Comparison of these data with excess molar volumes and factors governing on both mixtures shows that a main factor influencing the negative

excess volume of these mixtures is the structural effect. Indeed, the accommodation of MTBE molecules within the structure of alcohol molecules leads to the breakdown and collapse of their ordered structure, that decreases the volume of mixtures, and causes to the negative excess molar volume.

In addition, in refs. [2-5] values of excess molar enthalpy and excess molar volumes for MTBE + 1-alkanol are reported, and the influence of changing the alkyl chain on the properties mentioned is discussed. The same conclusion for increasing the alcohol chain length and its effect on the molecular interactions has been obtained indicating that the interactions become weaker as the length of the alcohol chain increases. Comparing the excess molar volumes of MTBE with 1-alkanol and 2-alkanol indicates that V_m^E for MTBE + 1-alkanol are also negative and greater (in absolute values) than reported data for MTBE + 2-alkanol. The displacement of the OH group from the first carbon to the second carbon (1-alkanol to 2-alkanol) causes a steric hindrance and prevents the ether molecules to form the strong bonds with alcohols and also their suitable fitting into the alcohols structure.

Deviation in viscosity $(\Delta\eta)$ was calculated by

$$\Delta\eta = \eta - x_1\eta_1 - x_2\eta_2 \tag{4}$$

η is the mixture viscosity, and η_i stands for the pure components. Values of $\Delta\eta$ for binary mixtures were correlated by the Redlich-Kister function, and A_k are reported in SI file, Table S2 alongside the standard deviation σ. Negative viscosity deviation for all the studied binary mixtures was obtained, and this behavior at $T = 298.15$ K is presented in Fig. 2. The viscosity deviations decrease in the sequence: 2-propanol < 2-butanol < 2-pentanol. By the addition of MTBE, the alcohol molecules dissociate and due to the reduction of their cohesive forces, have greater mobility than the pure state.

To further study the experimental densities of pure materials and binary systems, the PC-SAFT model was implemented. In this model [14,15] the residual Helmholtz energy is the starting point, and the other properties could be obtained from its derivations

$$a^{res} = a^{hc} + a^{disp} + a^{assoc} \tag{5}$$

The hard chain reference contribution is

$$a^{hc} = \bar{m}a^{hs} - \sum_i x_i(m_i - 1)\ln g_{ij}^{hs} \tag{6}$$

The mean segment number is represented by $\bar{m}$ and the pair distribution function by g_{ij}^{hs}

$$g_{ij}^{hs} = \frac{1}{1-\zeta_3} + \left(\frac{d_i d_j}{d_i + d_j}\right)\frac{3\zeta_2}{(1-\zeta_3)^2} + \left(\frac{d_i d_j}{d_i + d_j}\right)^2 \frac{2\zeta_2^2}{(1-\zeta_3)^3} \tag{7}$$

ζ_n is defined as

$$\zeta_n = \frac{\pi}{6}\rho\sum_{i=1}^n x_i m_i d_i^n \tag{8}$$

d_i is the segment diameter and usually temperature dependent

$$d_i = \sigma_i\left[1 - 0.12\exp\left(-\frac{3\varepsilon_i}{kT}\right)\right] \tag{9}$$

Hard sphere contribution a^{hs} is given by

$$a^{hs} = \frac{1}{\zeta_0}\left[\frac{3\zeta_1\zeta_2}{1-\zeta_3} + \frac{\zeta_2^3}{\zeta_3(1-\zeta_3)^2} + \left(\frac{\zeta_2^3}{\zeta_3^2} - \zeta_0\right)\ln(1-\zeta_3)\right] \tag{10}$$

a^{dis} is illustrated by

$$a^{dis} = -2\pi\rho I_1 \overline{m^2\varepsilon\sigma^3} - \pi\rho\bar{m}C_1 I_2 \overline{m^2\varepsilon^2\sigma^3} \tag{11}$$

The C_1 coefficient is calculated as

$$C_1 = \left[1 + \bar{m}\frac{8\eta - 2\eta^2}{(1-\eta)^4} + (1-\bar{m})\frac{20\eta - 27\eta^2 + 12\eta^3 - 2\eta^4}{[(1-\eta)(2-\eta)]^2}\right]^{-1} \tag{12}$$

where η is the reduced density, I_1 and I_2 are the perturbation integrals calculated by the power series in the density

$$I_1 = \sum_{i=0}^{6} a_i \eta^i \tag{13}$$

$$I_2 = \sum_{i=0}^{6} b_i \eta^i \tag{14}$$

T determine the cross parameters ε_{ij}, d_{ij} and σ_{ij} for pairs of unlike segments, the conventional combining rules were used

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j} \left(1 - k_{ij}\right) \tag{15}$$

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \tag{16}$$

$$d_{ij} = \frac{d_i d_j}{d_i + d_j} \tag{17}$$

k_{ij} is an adjustable parameter which corrects the dispersion forces in the mixtures. For associated compounds, a^{assoc} is determined by:

$$a^{assoc} = \sum_{i=1} x_i \left[\sum_{A_i} \left(\ln X^{A_i} - \frac{X^{A_i}}{2} \right) + \frac{1}{2} M_i \right] \tag{18}$$

The mole fraction of molecules not bonded at site A is presented by X^{Ai} and the association sites on the molecule with M_i. X^{Ai} depends on the molar density ρ_j and the association strength Δ^{AiBj}. Cross association parameters $\varepsilon^{A_iB_j}$ and $\kappa^{A_iB_j}$ for substances i and j are obtained by the simple combining rules

$$\varepsilon^{A_iB_j} = \frac{1}{2} \left(\varepsilon^{A_iB_i} + \varepsilon^{A_iB_j} \right) \tag{19}$$

$$\kappa^{A_iB_j} = \sqrt{\kappa^{A_iB_i} \kappa^{A_jB_j}} \left(\frac{\sqrt{\sigma_{ii}\sigma_{jj}}}{0.5\left(\sigma_{ii} + \sigma_{jj}\right)} \right)^3 \tag{20}$$

To calculate the density of the binary systems, at first, parameters of the PC-SAFT for the pure compounds should be computed. If the compounds are associated, five

parameters are needed; otherwise, three parameters are required. Calculation of these parameters is possible when their vapor pressure and liquid density are available. After obtaining the parameters of the pure materials, parameters for binary mixtures must be calculated. Except for ε_{ij} parameter, the rest of them are obtained by the mixing rules and Eqs. (15)-(20). Calculation of ε_{ij} requires an adjustable quantity k_{ij}, and its value is obtained from the iteration method when the predicted values have the closest amount to the experimental data. In fact, by defining an objective function, optimized values are obtained

$$\text{OF} = \sum_{i=1}^{N} \left(\frac{\Omega_i^{exp} - \Omega_i^{calc}}{\Omega_i^{exp}} \right)^2 \tag{21}$$

Here, Ω_i is the density of binary mixtures, and N stands for the number of experimental points. As stated in the original paper [12], the method for calculation of density is as follows: The density at a given pressure of the system P^{sys} is determined iteratively by adjusting the reduced density η until $P^{cal} = P^{sys}$. A suitable starting value for a liquid phase is $\eta = 0.5$ and values of $\eta > 0.74$ have no physical relevance. The number density of molecules ρ is calculated from η through

$$\rho = \frac{6}{\pi} \eta \left(\sum_i x_i m_i d_i^3 \right)^{-1} \tag{22}$$

Binary mixtures density was obtained by the method described here, and the values of parameter k_{ij} are presented in SI file, Table S3 along with standard deviations. Results of density calculation by this model for binary systems indicate that the correlation of density was accomplished with a good accuracy for all binary systems at $T = 298.15$ K as shown in Fig. 3.

CONCLUSIONS

For binary mixtures MTBE + short chain 2-alkanol, experimental values of density and viscosity at the temperature range of 293.15-323.15 K were reported. Negative values of excess molar volume and viscosity deviation were observed, and the non-ideality behavior of
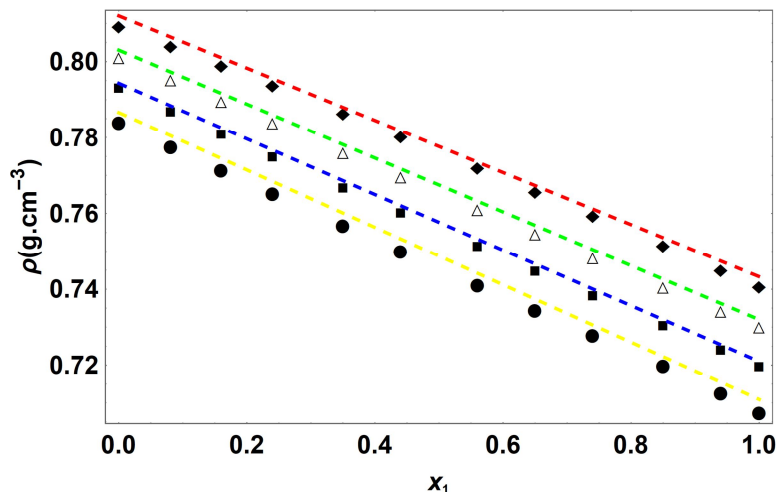
Fig. 3. Density for binary mixtures of methyl tert-butyl ether with 2-pentanol at (♦) 293.15 K, (Δ) 303.15 K, (■) 313.15 K, (●) 323.15 K. (----) PC-SAFT.

systems decreased with increasing temperature. Results show that the structure of MTBE/Alkan-2-ol solvents is governed mainly by the formation of H-bonds, geometrical structure, and size of the components. The PC-SAFT theory was tested for its correlative ability to calculate the binary densities. Results show that this model can correlate the experimental data with a reasonable agreement for all investigated systems. Minimum of deviations between experimental densities and calculated values by the PC-SAFT model is 1.1% and for MTBE + 2-propanol while the maximum of deviation is 1.4% and belongs to the binary mixtures MTBE + 2-butanol.

ACKNOWLEDGMENTS

APPENDIX A. SUPPLEMENTARY DATA

Supplementary data associated with this article can be found, in the online version, at http://

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