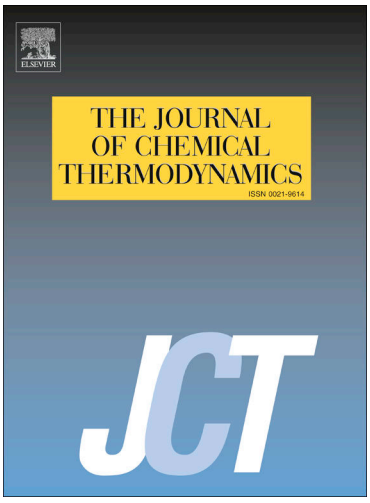
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Thermophysical properties of Binary Liquid Mixtures of Oxygenated Compounds: 2-Methoxyethanol + Alcohols at T = 298.15 K and 313.15 K

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Abstract

Thermophysical properties as density, (ρ), dynamic and kinematic viscosities, (η, υ), refractive index, (n_D), and excess enthalpy, (H^{E}), are presented in this present work for binary mixtures containing 2-methoxyethanol, 1-butanol, 2-butanol, and 1-propanol at T = (298.15 and 313.15) K and at p = 0.1 MPa, over the whole range of composition. Derivative properties such as excess volume, (V^E), and deviations in refractive index, (Δn_D), were calculated from the measured data of density and refractive index, respectively. The Perturbed Chain-Statistical Associating Fluid (PC-SAFT) Equation of State is used to correlate the experimental data density for the studied binary mixtures. Also, the Redlich-Kister equation is employed to fit the excess volumes, deviations in refractive index, and excess enthalpies. Besides, the NRTL and UNIQUAC models are applied to correlate the measured data of

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excess enthalpy, (H^E). Moreover, intermolecular interactions have been discussed for the studied binary mixtures.

Keywords

Oxygenated Compound; Density; Dynamic and Kinematic Viscosity; Excess Enthalpy; Refractive Index; PC-SAFT EoS.

1. Introduction

The use of fossil fuels has shown harmful environmental effects, which led to many studies to search for alternatives to reduce the environmental aspect of fuels. Adding different oxygenated additives to fuel (fuel reformulation) is one of the proposed alternatives that improve the combustion in engines, and therefore reduce pollutant emissions (CO, NO_x, unburnt hydrocarbons, and smoke) and increase engine efficiency. Some authors [1] have demonstrated that there is a relation between the decreases in particulate emissions and the percentage of oxygen in the mixture. The used oxygenated additives are mostly methyl esters, derived from vegetable oils and ethanol. However, other oxygenated organic compounds (glycol ethers, ethers, hydrogenated monoterpenes, other alcohols, and esters, etc.) have been studied to determine their effect on fuel properties, combustion, and emissions. Some of them have significantly revealed considerable effects on decreasing the toxicity of emissions and on fuel properties and combustion. Multiple researchers [2] have worked on mixtures of glycol ethers with diesel fuel, which demonstrates an important decrease in emissions of CO, unburnt hydrocarbons, and the mass of opaque soot. Also, these results showed that mixing oxygen with glycol ether was more efficient than mixing oxygen with alcohol [3].

The glycol ethers are composed of hydrocarbon bonded with both ether and alcohol. These dual functional groups in the same molecule, with both non-polar and polar properties, give versatile solvency characteristics. Glycol ethers are used for various applications, especially industrial solvents. Also, they are applied as additives to diesel fuel [2]. Moreover, Alkanols

have an extremely wide field of industrial applications, especially in the manufacturing of fuels, perfumes, cosmetics, paints, drugs, explosives, fats, waxes, resins, plastics, and more [4 and 5]. 2-Methoxyethanol represents in this work the glycol ethers group, and 1-butanol, 2-butanol and 1-propanol represent the alkanols group. This work is the continuation of our previous studies regarding the thermophysical properties of n-alkoxyethanol + hydrocarbon / + alcohol mixtures already published [6-12].

There is a large growing era of research to find new sources of energy for industrial uses, and also the optimum way to their exploitation. Between the industrial applications needs and developing new energy sources as clean as possible, it is required to have comprehensive and full knowledge in the field of thermodynamics, to do a better selection of the systems that have the minimum environmental impact. Therefore, it is essential to study the thermo physical properties of these new systems, which should be determined through experimental research and the development of scientific models that more or less adhere to experimental results and predict their behaviour for other conditions. Besides, these thermophysical properties determined by experimental research could be a good asset for the development and verification of various theories and models of these systems.

The main objective of this present work is to determine experimental data of thermophysical properties for binary mixtures: (*i*): 2-methoxyethanol (1) + 1-butanol (2), (*ii*): 2-methoxyethanol (1) + 2-butanol (2), and (*iii*): 2-methoxyethanol (1) + 1-propanol (2), at (298.15 and 313.15) K and at 0.1 MPa, and also at various mole fractions. The experimental thermophysical properties reported in this work are: density, (ρ), dynamic and kinematic viscosities, (η, υ), refractive index, (n_D), excess enthalpy, (H^{E}), and derivatives properties such as excess volume, (V^E), and deviations in refractive index, (Δn_D). Measured data of density for the studied binary mixtures have been modelled by using the Perturbed Chain-Statistical Associating Fluid (PC-SAFT) equation of state [13,14]. Also, the Redlich-Kister

equation [15] is employed to fit the excess volumes, deviations in refractive index, and excess enthalpies. Besides, the NRTL [16] and UNIQUAC [17] models are applied to correlate the measured data of excess enthalpy, (H^E). Besides, intermolecular interactions have been discussed for the studied binary mixtures.

2. Experimental

2.1. Chemicals

The chemicals employed in these experiments are 2-methoxyethanol, 1-butanol, 2-butanol, and 1-propanol. The chemicals were selected with high state mole fraction purity values (>0.990), to obtain good and reliable experimental results. Table 1 shows the chemical properties of the studied compounds, and Table 2 presents a comparison of density, (ρ), dynamic viscosity, (η), and refractive index, (n_D), with some reported data previously published in the literature [18-68], which demonstrates a good agreement compared to literature data. Using an OHAUS analytical balance with a precision of 0.0001g, the preparation of binary mixtures containing 2-methoxyethanol, 1-butanol, 2-butanol, and 1-propanol was done by mass. 0.0005 is the estimated uncertainty for the mole fraction.

2.2. Apparatus and procedure

2.2.1. Density, dynamic and kinematic viscosities, and Refractive Index

A Stabinger SVM 3000 viscosimeter was used in the present work to measure densities (ρ), dynamic and kinematic viscosities, (η, υ), at (298.15 and 313.15) K and 0.1 MPa for pure compounds (2-methoxyethanol, 1-butanol, 2-butanol, and 1-propanol) and their binary mixtures. This apparatus consists of two rotating concentric tubes. Its operating mode is based on the principle of Couette that states that the viscosity is proportional to the torque difference between the rotating cylinders. Apparatus performs five measurements automatically with a relative uncertainty of the viscosity 2% (k = 2), and the expanded uncertainties of density, temperature, and mole fraction are respectively, $5 \cdot 10^{-4}$ g.cm^{-3} (k = 2, level of confidence

95.45%), 0.04 K and 0.0005. An Abbe digital refractometer (Model Abbemat 300, Anton Paar) was used to measure the refractive index of the pure components and their binary mixtures. The expanded uncertainty of the refractive index is equal to 0.005. The Stabinger SVM 3000 viscosimeter is calibrated using air and decane, while, the Abbe digital refractometer is calibrated using air and water.

2.2.2. Excess Enthalpy H^E

Excess enthalpy, H^E, measurements were carried out using an isothermal flow calorimeter already described in the previous paper [69]. The fluids composing the mixture (2-methoxyethanol + 1-butanol, or + 2-butanol, or + 1-propanol) are injected by two pumps through two stainless steel tubes with a programmable flow into the mixing chamber in the measuring cell. The measuring cell is immersed in a thermostatic bath and it is in charge to maintain the cell temperature at the desired value. The temperature stability obtained using a thermostatic system is higher than 0.01 K. The flow rates, the molecular weights, and the densities of each liquid (Tables 1 and 2) are three sufficient properties to determine different mole fraction (x_i) of the studied binary mixtures [2-methoxyethanol (1) + 1-butanol (2), 2-methoxyethanol (1) + 2-butanol (2) and 2-methoxyethanol (1) + 1-propanol (2)] with an expanded uncertainty $u(x)$ = 0.0005. Afterward, it permits determining the excess enthalpy, H^E, for each specific mole fraction. To do this, the excess enthalpy, H^E, is acquired by the following equation: $H^E = \frac{Q_{mixture}}{\dot{n}_{mixture}}$, where $Q_{mixture}$ is the heat of mixing and $\dot{n}_{mixture}$ is the number of moles per second. The relative expanded uncertainty (k = 2) U_r (H^E) = 1% for excess enthalpy H^E.

3. Correlation of Excess Enthalpy H^E:

The modified Redlich-Kister equation [15] is a relevant equation to fit the values of excess enthalpy, H^E, for each binary mixture and it is given by the following expression:

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$$H^{E} = \frac{x \cdot (1-x) \cdot \sum_{i=1}^{n} A_i \cdot (2x-1)^{i-1}}{1 + A_0 \cdot (2x-1)} \quad (1)$$

Where; x: the mole fraction, A_i: Redlich-Kister coefficients; and they are calculated using the unweighted least-squares method. The optimal number of A_i was obtained by employing the *F*-test [70].

4. Modeling of Excess Enthalpy, H^E, with NRTL and UNIQUAC Models:

4.1. NRTL model

The first model used to correlate the excess enthalpy, H^E, data of the studied binary mixtures is the NRTL model [16], and it is giving by the following equation:

$$H^{E} = -RT\sum_{i=1}^{n} x_i \eta_i \quad (2)$$

Where; x_i: Composition of component *i*; and η_i is obtained by the following equation:

$$\eta_i = \frac{\sum_{k=1}^{p} x_k \tau_{ki} G_{ki} \left[\alpha \left(\tau_{ki} - \left(\sum_{n=1}^{p} x_n \tau_{ni} G_{ni} \Big/ \sum_{l=1}^{n} x_l G_{li} \right) \right) - 1 \right]}{\sum_{l=1}^{p} x_l G_{li}} \quad (3)$$

$$G_{ji} = \exp\left(-\alpha \tau_{ij}\right) \quad (4)$$

$$\tau_{ij} = (g_{ij} - g_{ii})/RT \quad (5)$$

Where; g_{ji}: Interaction energy between each pair of *i-j* molecules; α: Non-randomness factor in the mixture; *x*: Mole fraction. About NRTL theory, the excess enthalpy, H^E, of a multi-component mixture relies on binary parameters. In this work, the non-randomness parameter α is considered as an adjustable parameter for the three-parameter.

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4.2. UNIQUAC model

The second model employed for the correlation of H^E data of the studied binary mixtures is the UNIQUAC model [17], and it is given by the following expression:

$$H^E = \sum_{i=1}^{n} q_i x_i \frac{\sum_{j=1}^{n} \vartheta_j \Delta u_{ji} \tau_{ji}}{\sum_{j=1}^{n} \vartheta_j \tau_{ij}} \tag{6}$$

Where; $\vartheta_i = \frac{q_i x_i}{\sum_j q_j x_j}$ and q_i is the molecular surface area, calculated by summing the contributions of the functional groups composing the compound.

To obtain a reliable and effective study on the experimental excess enthalpy, H^E, data, we compared the experimental H^E data with those obtained by the Redlich-Kister equation, NRTL, and UNIQUAC models, different deviation parameters have been applied, such as root mean square deviation, *rms*, absolute difference maximum, max $|\Delta H^E|$, maximum relative deviation, max $(|\Delta H^E|/H^E)$, and absolute average deviation, AAD, which are calculated by the following equations:

$$rms = \left[\frac{\sum_{i=1}^{N} \left(H^E_{exp} - H^E_{calc}\right)^2}{N - n_{\text{par}}}\right]^{1/2} \tag{7}$$

$$\max|\Delta H^E| = max\left|H^E_{\text{exp}} - H^E_{\text{calc}}\right| \tag{8}$$

$$\max\left(|\Delta H^E|/H^E\right) = max\left(\frac{\left|H^E_{\text{exp}} - H^E_{\text{calc}}\right|}{H^E_{\text{exp}}}\right) \tag{9}$$

$$AAD = \frac{100}{N}\sum_{i=1}^{N}\left|\frac{H^E_{exp} - H^E_{calc}}{H^E_{exp}}\right| \tag{10}$$

Where; H^E_{exp}: Experimental data of H^E; H^E_{calc}: Calculated values of H^E using different equations and models; N: Number of measured data; n_{par}: Number of parameters for the used equation or model.

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5. Correlation and modeling of density, dynamic and kinematic viscosities, refractive index, and derivative properties

5.1 Correlation

Density, (ρ), dynamic and kinematic viscosities, (η, υ), and refractive index, (n_D), for binary mixtures are fitted using a mathematical polynomial equation, expressed as follows:

$$P(x) = \sum_{i=1}^{N} A_i . x^{i-1} \quad (11)$$

Where; P function could be density, (ρ), dynamic viscosity, (η), kinematic viscosity, (υ), or refractive index, (n_D); x is the mole fraction; A_i coefficients are determined using the unweighted least-squares method. Using the *F*-test [70], the optimal number of A_i was selected. The sets of coefficients A_i used to fit the measured data of density, (ρ), dynamic viscosity, (η), kinematic viscosity, (υ), and refractive index, (n_D), are enumerated in Table 3. Derivative properties as excess volume, (V^E), or deviations in refractive index, (Δn_D), are correlated using the following Redlich-Kister equation [15]:

$$Q(x) = x.(1-x).\sum_{i=1}^{N} A_i.(2x-1)^{i-1} \quad (12)$$

Q function could be excess volume, (V^E), or deviation in refractive index, (Δn_D), x is the mole fraction and A_i coefficients are determined using the unweighted least-squares method. Also, the sets of adjustable coefficients A_i needed to correlate excess volume, (V^E), and deviations in refractive index, (Δn_D), at each temperature are reported in Table 4, with the corresponding root-mean-square deviations σ:

$$\sigma(X) = \left[\sum_{i=1}^{N} \frac{(X_{exp} - X_{calc})^2}{(N-p)}\right]^{1/2} \quad (13)$$

With; N: the number of measured data; p: the number of parameters employed in the Redlich-Kister equation.

5.2 Modelling

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The PC-SAFT (Perturbed-Chain for Statistical Associating Fluid Theory) is a molecular-based thermodynamic model [13,14], that uses hard chains formed by spherical particles as reference fluid.

The equation of state (PC-SAFT) is equivalent to the residual Helmholtz free energy a^{res}, composed of different types of intermolecular interactions, including terms for the hard chain reference a^{hc}, the dispersion interactions a^{disp} and the association interaction a^{assoc}:

$$\breve{a}^{res} = \breve{a}^{hc} + \breve{a}^{disp} + \breve{a}^{assoc} \tag{14}$$

At first, Wertheim and Chapman [71, 72] started by defining hard chains reference term noted as a^{hc} and constituted by $\overline{m}$ segments, shown as follows:

$$\breve{a}^{hc} = \overline{m}\breve{a}^{hc} - \sum_{i=1}^{n_c} x_i(m_i - 1) ln g_{ij}^{hs} \tag{15}$$

Where; x_i: Mole fraction of the chain of compound i; m_i: Number of segments in the chain; g_{ij}^{hs}: Radial distribution function for the segments of the compounds i and j in a system of hard spheres.

Also, the dispersion interaction term, a^{disp}, of PC-SAFT equation has been determined by Barker and Henderson's perturbation theory [73,74], expressed by the following equation:

$$\breve{a}^{disp} = -2\pi\breve{\rho}I_1\overline{m^2\varepsilon\sigma^3} - \pi\breve{\rho}C_1I_2\overline{m^2\varepsilon^2\sigma^3} \tag{16}$$

Where; C_1: Coefficient that relies on the mean segment number $\overline{m}$ and on the density number of the fluids ρ and the perturbation integral I_1 and I_2.

Moreover, Chapman and Huang [75-77] developed the association interaction expression defined as follows:

$$\breve{a}^{assoc} = \sum_{i=1}^{n_c} x_i\left[\sum_{A_i}\left(lnX^{A_i} - \frac{X^{A_i}}{2}\right) + \frac{1}{2}M_i\right] \tag{17}$$

Where; M_i: Association sites number on each molecule; X^{A_i}: Composition of molecules I not linked at site A; $\sum_{Ai}$: a sum of all associating sites on each molecule.

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The PC-SAFT equation of state is characterized by various terms, the segment number formed by non-associative parameters(m), the segment energy parameter (ε/k), and the segment diameter (σ). In the case of the non-ideal solutions, the association interaction term in equation (4) has to be divided into two other parameters, the association volume (k^{AiBi}) and the association energy (ε^{AiBi}).

The PC-SAFT parameters of the studied binary systems were characterized by employing the objective function noted as $Obj.F$:

$$Obj.F = \sum_{i=1}^{N} \left(\frac{\rho_i^{exp} - \rho_i^{calc}}{\rho_i^{exp}} \right) \quad (18)$$

Where; N: Number of measured data.

Table 5 shows the PC-SAFT equation of state parameters for each studied pure component (2-methoxyethanol, 1-butanol, 2-butanol, and 1-propanol) and the average absolute deviations (AAD) between the experimental densities and modelled data from the PC-SAFT equation of state. The AAD_s obtained for 2-methoxyethanol, 1-butanol, 2-butanol and 1-propanol were 0.014%, 0.030%, 0.040% and 0.006%, respectively.

6. Results and Discussion

Thermophysical properties such as density, (ρ), dynamic and kinematic viscosities, (η, υ), refractive index, (n_D), and excess enthalpy, (H^E), for the binary mixtures 2-methoxyethanol (1) + 1-butanol (2), + 2-butanol (2), and + 1-propanol (2), are reported at different compositions, at 0.1 MPa and at (298.15 and 313.15) K.

6.1. Excess enthalpy H^E

Excess enthalpy, (H^E), measured data for the studied binary mixtures: 2-methoxyethanol (1) + 1-butanol (2), + 2-butanol (2), and + 1-propanol (2), are listed in Table 6 and presented in Figures 1, 2, and 3. The sets of parameters needed for the calculation of H^E by the modified Redlich-Kister equation, NRTL, and UNIQUAC models, are presented in Tables 7 and 8.

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The first binary mixture 2-methoxyethanol (1) + 1-butanol (2) was measured at T = (298.15 and 313.15) K. The maximum value of H^E is 633.7 J.mol^{-1} at 298.15 K and 704.2 J.mol^{-1} at 313.15 K, both of them at the same mole fraction (x_1 = 0.50). At 298.15 K, the best fit of H^E data is obtained with the modified Redlich-Kister equation, with a root mean square deviation, rms ΔH^E, of 1.2 J.mol^{-1}. NRTL and UNIQUAC models present also a good fit with a root mean square deviation, rms ΔH^E, of 2.5 J.mol^{-1} and 4.9 J.mol^{-1}, respectively. While, at 313.15 K the best fit is obtained with the NRTL model with a root mean square deviation, rms ΔH^E, of 1.1 J.mol^{-1}. Modified Redlich-Kister equation and UNIQUAC model show also a good fit with a root mean square deviation, rms ΔH^E, of 1.4 J.mol^{-1} and 3.9 J.mol^{-1}, respectively. This present binary mixture shows an endothermic behavior (H^E>0) throughout the whole range of mole fractions (Figure 1). At 298.15 K, our experimental data of excess enthalpy for the studied binary mixture 2-methoxyethanol (1) + 1-butanol (2) were compared with data reported by Cobos et *al.* [78] and Reddy et *al.* [79], this comparison (Figure 1) shows that our experimental data agree within 7.5% and 6.1%, respectively. While, at 313.15 K, no reference data were found in the literature for comparison with our reported data of excess enthalpy.

The second binary mixture 2-methoxyethanol (1) + 2-butanol (2) was also studied at 298.15 and 313.15 K, and shows also an endothermic behavior (Figure 2) with a maximum value of H^E of 822.7 J.mol^{-1} and 771.0 J.mol^{-1}, at (298.15 and 313.15) K and the mole fractions x_1 = 0.45 and x_1 = 0.50, respectively. The modified Redlich-Kister equation was also the best-adapted correlation equation at 298.15 K for excess enthalpy data with a root mean square deviation, rms ΔH^E, of 1.5 J.mol^{-1}. NRTL and UNIQUAC models present a good agreement with a root mean square deviation, rms ΔH^E, of 2.1 J.mol^{-1} and 4.5 J.mol^{-1}, respectively. Besides, at 313.15 K, the UNIQUAC model presents a good agreement with a root mean square deviation, rms ΔH^E, of 1.7 J.mol^{-1}. Modified Redlich-Kister equation and NRTL model show a good agreement with a root mean square deviation, rms ΔH^E, of 2.1 J.mol^{-1} and 3.8

J.mol^{-1}. No reference data were found in the literature for the present binary mixture 2-methoxyethanol (1) + 2-butanol (2) at the studied temperatures.

The third binary mixture 2-methoxyethanol (1) + 1-propanol (2) presents also an endothermic behavior with a positive sign of H^E over the whole range of mole fraction and at T = (298.15 and 313.15 K) (Figure 3). This binary mixture shows also a high value of H^E, where the maximum value of H^E is 541.2 J.mol^{-1} at 298.15 K and 570.1 J.mol^{-1} at 313.15 K and the same mole fraction x_1 = 0.45. Modified Redlich-Kister equation presents the best fit of H^E measured data at both studied temperatures (298.15 and 313.15) K, with the same values of the root mean square deviation, rms ΔH^E, of 0.6 J.mol^{-1}. NRTL and UNIQUAC models shows also a good agreement at both temperatures. Our H^E experimental data for this binary mixture 2-methoxyethanol (1) + 1-propanol (2) at 298.15 K agree within 6.3 % with data reported by Reddy et *al.* [79]. Besides, at 313.15 K, no reference data were found in the literature for comparison. Our experimental data for the studied binary are compared graphically with data measured at 321.15 K that are reported by Chandak et *al.* [92]. And it can be noticed in Figure 3, that data reported by this author follow the same trend when the temperature increases, such as excess enthalpy increases with increasing temperature.

The term excess enthalpy, H^E, is very useful to comprehend the nonideality of the final mixture solution. This concept is one of the enthalpic effects, caused by shape and size differences between distinct molecules and the various interactions between them, which could lead to either the increase or the drop of H^E [80]. In this context, all the studied binary mixtures: 2-methoxyethanol (1) + 1-butanol (2), + 2-butanol (2), and + 1-propanol (2), reveal an endothermic behaviour (H^E>0) at both studied temperatures (298.15 and 313.15) K and throughout the entire range of mole fraction. It was expected to observe this behaviour for the studied binary mixtures, due to the breaking of intermolecular hydrogen bonds while mixing

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of 2-methoxyethanol as a glycol ether with the different alcohols (1-butanol, 2-butanol, and 1-propanol).

The comparison between the three studied binary mixtures 2-methoxyethanol (1) + 1-butanol (2), + 2-butanol (2) and + 1-propanol (2) demonstrates that for the given 2-methoxyethanol, the values of excess enthalpy H^E at both temperatures 298.15 and 313.15 K changed in the following order: 1-propanol < 1-butanol < 2-butanol. The comparison between the three studied binary mixtures shows a minor variation in H^E quantity between 298.15 and 313.15 K, where the first binary mixture (2-methoxyethanol (1) + 1-butanol (2)) has 70.5 J.mol^{-1} as a difference in H^E quantity between 298.15 and 313.15 K, the second binary mixture (2-methoxyethanol (1) + 2-butanol (2)) has 51.7 J.mol^{-1} as a difference in H^E quantity between the studied temperatures, also the difference in H^E quantity between both 298.15 and 313.15 K for the third binary mixture (2-methoxyethanol (1) + 1-propanol (2)) is 28.9 J.mol^{-1}, this small difference in H^E quantity between the studied temperatures (298.15 and 313.15 K) for the three studied binary mixtures is due to the similarity in the type of surface for each alcohol (1-butanol , 2-butanol or 1-propanol), even though the maximum values of excess enthalpy for the three binary mixtures 2-methoxyethanol (1) + 1-butanol (2), + 2-butanol (2), and + 1-propanol (2) were [633.7 J.mol^{-1} - 704.2 J.mol^{-1}], [822.7 J.mol^{-1} – 771.0 J.mol^{-1}] and [541.2 J.mol^{-1} – 570.1 J.mol^{-1}] at 298.15 and 313.15 K, respectively.

The excess enthalpy versus mole fraction curves are nearly symmetric in all the studied binary mixtures (2-methoxyethanol (1) + 1-butanol (2), 2-methoxyethanol (1) + 2-butanol (2) and 2-methoxethanol (1) + 1-propanol (2)). The excess enthalpy of these binary mixtures may be influenced by factors such as (*i*) absorption of heat due to depolymerization of self-associated alcohols or 2-methoxyethanol, and (*ii*) liberation of heat as a result of possible hydrogen bonding interaction between the ether group of the alkoxyethanol (2-methoxyethanol) and the hydroxyl function of the alcohol (1-butanol, 2-butanol or 1-propanol) [79]. The actual values

of excess enthalpy H^E would depend upon the relative strength of the two opposing effects. The positive experimental H^E values suggest that the first effect is stronger than the second in all the studied binary mixtures [79].

6.2. Density, ρ, dynamic and kinematic viscosities, (η, υ), refractive index, (n_D), and refractive index n_D

It is more significant to search for several thermophysical properties such as density, dynamic and kinematic viscosities, and refractive index to understand the nature of different molecular interactions between various binary mixtures. For this reason, density, (ρ), dynamic and kinematic viscosities, (η, υ), refractive index, (n_D), were reported at (298.15 and 313.15) K and 0.1 MPa for the binary mixtures: 2-methoxyethanol (1) + 1-butanol (2), + 2-butanol (2) and + 1-propanol (2), and are listed in Table 9 and plotted in Figures 4, 5, 6 and 7. Figures 4 and 7 respectively show that the values of density, (ρ), and refractive index, (n_D), decrease when the temperature increases from 298.15 and 313.15 K and increase with the augmentation of the concentration x_1 for all the studied binary mixtures. While, as shown in Figures 5 and 6, dynamic and kinematic viscosities, (η, υ), values of the studied binary mixtures decrease also while increasing the temperature from 298.15 to 313.15 K and a decline with the augmentation of concentration for all the studied binary mixtures. Experimental data of density for the binary mixtures 2-methoxyethanol (1) + 1-butanol (2) and + 1-propanol (2) studied in the present work are compared with data previously published by Roy et *al*. [81], Zarei et *al.* [82], Mozo et *al*. [83] and Pal et *al.* [90] for the same binary mixtures. The comparison shows a good agreement for the first binary mixture (2-methoxyethanol (1) + 1-butanol (2)) with Roy et *al*. [81] and Mozo et *al*. [83] with an AAD at 298.15 K of 0.15% and 0.05%, respectively, also the comparison demonstrates a good agreement for the second binary mixture (2-methoxyethanol (1) + 1-propanol (2)) with Roy et *al*. [81], Zarei et *al.* [82] and Pal et *al.* [90], with an AAD at 298.15 K of 0.20% (with Roy et

al. [81]) and 0.03% (with Pal et *al.* [90]), while at 313.15 K, the AAD was 0.04% as a comparison between our density data and data reported by Zarei et *al.* [82]. Our density experimental data for the three studied binary mixtures are compared graphically with data measured at different temperatures which are different to our measuring range and reported by Pal et *al.* [93], Reddy et *al.* [94] and Krishnan et *al.* [95]. It can be noticed in Figure 4, that these reported data follow the same trend when the temperature increases or decreases, such that the density decreases with increasing temperature and increases with decreasing temperature. Also, dynamic viscosity experimental data reported at 298.15 K in this work for binary mixtures 2-methoxyethanol (1) + 1-butanol (2) and + 1-propanol (2) were compared to data reported by Roy et *al*. [81] and Pal et *al.* [90], for the first binary mixture, the AAD value between our reported data and data reported by Roy et *al*. [81] was 4.39 %, while for the second binary mixture the comparison with data reported by Roy et *al*. [81] and Pal et *al.* [90] shows an AAD values of 3.62% and 1.14%, respectively. For the third studied binary mixture 2-methoxyethanol (1) + 2-butanol, no reference data were found in the literature to compare with them our density and dynamic viscosity data for the same binary mixture and the same experimental conditions (temperature and pressure). While, some dynamic viscosity reported data by Pal et *al.* [93], Reddy et *al.* [94] and Krishnan et *al.* [95] for the studied three binary mixtures that are measured at different temperatures which are different to our measuring range of temperature, they are compared graphically with our experimental data as shown in Figure 5, and we notice that these reported data follow the same trend when the temperature increases or decreases, such as dynamic viscosity decreases with increasing temperature and increases with decreasing temperature. Kinematic viscosity data for binary mixture 2-methoxyethanol (1) + 1-propanol (2) measured in this work at 313.15 K are compared with data reported by Chandak et *al.* [92] at the same temperature, and a good agreement has been noticed (Figure 6-c) with an AAD equals to 1.1%. Besides, no references were found in

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literature database to compare with them our experimental data of kinematic viscosity for the other studied binary mixtures at different temperatures. Figure 4 shows also the correlated densities by using the PC-SAFT equation of state and the results demonstrate a good agreement for all the studied binary mixtures compared with experimental data. In addition, the AAD values for the studied binary mixtures 2-methoxyethanol (1) + 1-butanol (2), + 2-butanol (2) and + 1-propanol (2) at 298.15 and 313.15 K are respectively within [0.28% - 0.27%], [0.26% - 0.25%] and [0.66% - 0.62%]. The comparison between the modelled values of density using the PC-SAFT equation of state and the experimental data presents a good agreement, due to the effect that the PC-SAFT EoS has a basis in statistical mechanics that considers the size and shape of the molecules [84-89]. Also, the association is explicitly considered in the PC-SAFT EoS, which is important to model the binary mixtures presented in this work.

6.3. Excess volume V^E

The calculation of excess volumes, (V^E), for the studied binary mixtures 2-methoxyethanol (1) + 1-butanol (2), + 2-butanol (2) and + 1-propanol (2), was done employing the following equation:

$$V^E = \sum_{i=1}^{n} x_i M_i \left[\left(1/\rho \right) - \left(1/\rho_i \right) \right] \tag{19}$$

Where; M_i: Molar mass for component *i*; x_i: Mole fraction for component *i*; ρ_i: Density for component *i*; ρ: Density of the studied binary mixture.

Figure 8 shows the excess volume, V^E, variations at 298.15 and 313.15 K depending on the mole fraction x_i for the studied binary mixtures: 2-methoxyethanol (1) + 1-butanol (2), + 2-butanol (2) and + 1-propanol (2). It was further observed in Figure 8 that excess volume, V^E, values are positive for all studied binary mixtures 2-methoxyethanol + alkanols (1-butanol, 2-butanol, or 1-propanol) all over the entire range of mole fraction, and this figure presents a

growing tendency of excess volume, V^E, while increasing the temperature from 298.15 to 313.15 K. Excess volume values, V^E, obtained are resulting from various opposing effects. The differences in the self-association (inter- or intramolecular) of glycol ether (2-methoxyethanol) and physical interactions that occur between glycol ether molecules (2-methoxyethanol) or alcohol molecules (1-butanol, 2-butanol, or 1-propanol) engender an increase of V^E with the variation of temperature from 298.15 to 313.15 K. For all the studied binary mixtures: 2-methoxyethanol + 1-butanol, + 2-butanol, or + 1-propanol, the excess volume, V^E, shows positive values, because of the hydrogen bond breaking mechanism of 2-methoxyethanol as an alkoxyethanol compound and 1-butanol, 2-butanol or 1-propanol as an alkanol compound in the pure state on mixing. The representative curves of excess volume, V^E, for all the studied binary mixtures have a parabolic shape almost symmetrical in the mole fraction x = 0.50. The results of excess volume, V^E, are significantly influenced by the temperature conditions, which proves the dependence between the two properties. Figure 8 demonstrates that the values of V^E increase with the elevation of temperature for all the studied binary mixtures, which can be justified by the weakening of hydrogen bonds at high temperatures. A good agreement is noticed in Figure (8-a) between our calculated V^E values and calculated values by Cobos et *al.* [91] for the binary mixture 2-methoxyethanol + 1-Butanol. While, for the binary mixture 2-methoxyethanol + 1-propanol, the comparison between our calculated V^E values and calculated values by Pal et *al.* [90] and Chandak et *al.* [92] shows a worse agreement (Figure 8-c) at 298.15 and 313.15 K, respectively.

6.4. Deviation in refractive index Δn_D

The deviations in refractive index, Δn_D, were determined by employing the following equation:

$$\Delta n_D = n_D - \sum_{i+1}^{N} x_i n_{Di} \quad (20)$$

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Where; n_i: Refractive index of pure component i; and n_D: Refractive index of the binary mixture. The calculated values of deviation in refractive index, Δn_D for all the studied binary mixtures at 298.15 and 313.15 K are plotted in Figure 9. As shown in Figure 9, the calculated values of deviation in refractive index, Δn_D, are all negative for the binary mixtures: 2-methoxyethanol (1) + 1-butanol (2) and + 2-butanol (2), over the whole range of mole fraction and at both studied temperatures (298.15 and 313.15) K. Besides, for the binary mixture 2-methoxyethanol (1) + 1-propanol (2), Δn_D values are all positive at 298.15 K, whereas, at 313.15 K, Δn_D values are both positive (poor region of 2-methoxyethanol) and negative (rich region of 2-methoxyethanol), as a result of the steric hindrance effect between unlike molecules of 2-methoxyethanol and 1-propanol as shown in Figure 9.

7. Conclusions

New data of density, (ρ), dynamic and kinematic viscosities, (η, υ), refractive index, (n_D), and excess enthalpy, (H^{E}), are reported for binary mixtures containing 2-methoxyethanol with 1-butanol or 2-butanol or 1-propanol at (298.15 and 313.15) K and 0.1 MPa and over a wide range of composition. Derivative properties as excess volume, V^E, and deviations in refractive index, Δn_D, are also calculated from the reported experimental data. PC-SAFT equation of state used to predict results of density showed good predictive capability. Intermolecular interaction effects are discussed for all studied binary mixtures.

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LIST OF SYMBOLS

H^E; Excess enthalpy, ρ; Density, (η); Dynamic viscosity, (υ); Kinematic viscosity, n_D; Refractive index, V^E; Excess volume, Δn_D; Deviation in refractive index, EoS; Equation of State, T; Temperature, p; Pressure, x_i; Mole fraction, i; Constituent identification.

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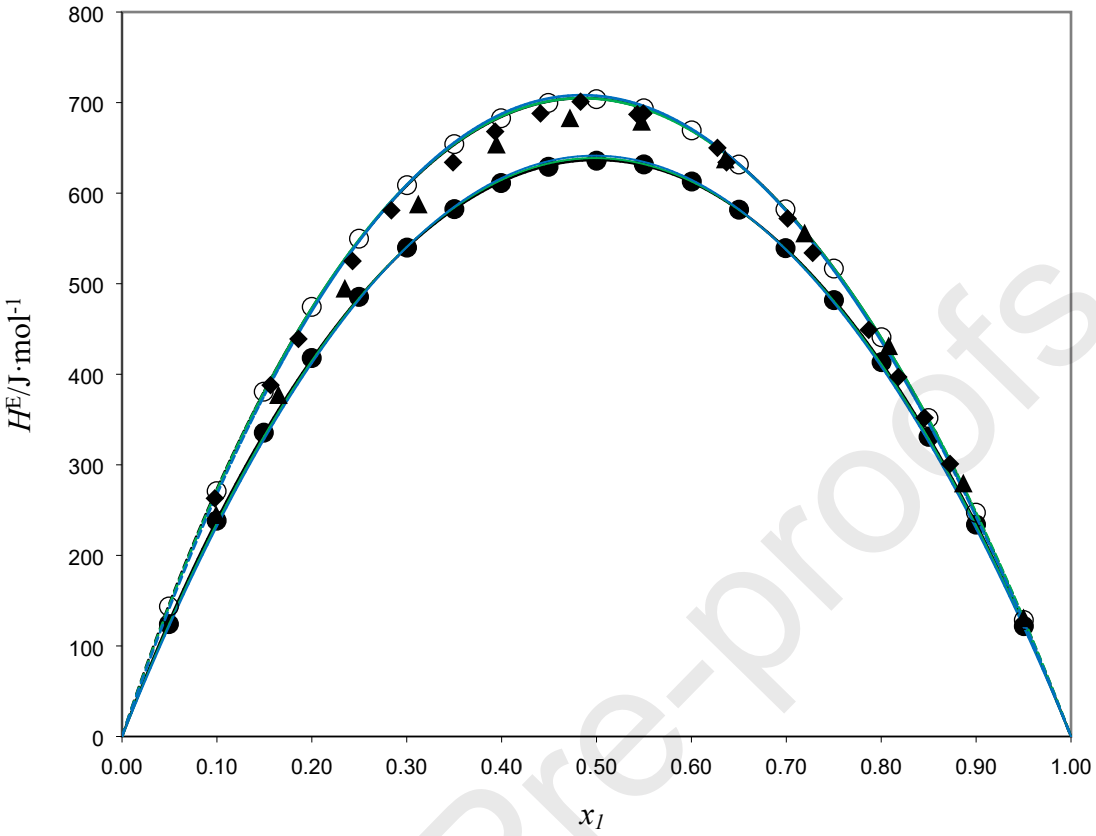


Figure 1. Excess enthalpy H^E of 2-methoxyethanol (1) + 1-butanol (2). At T = 298.15 K: (●), experimental data; (♦), Cobos et *al.* [78]; (▲), Reddy et *al.* [79]; (——), calculated values with modified Redlich-Kister equation; (——), calculated values with NRTL model; (——), calculated values with UNIQUAC model. At T = 313.15 K: (○),experimental data; (----), calculated values with modified Redlich-Kister equation; (----), calculated values with NRTL model; (----), calculated values with UNIQUAC model.

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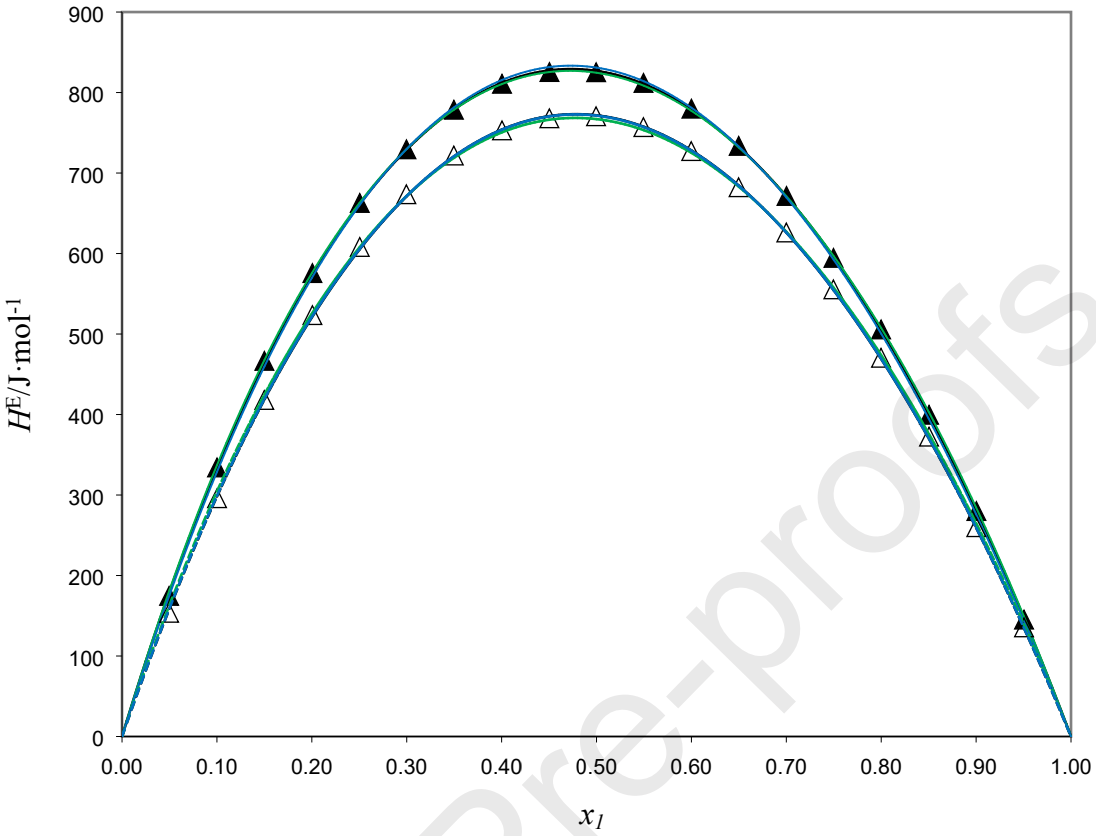


Figure 2. Excess enthalpy H^E of 2-methoxyethanol (1) + 2-butanol (2). At T = 298.15 K: (▲), experimental data; (——), calculated values with modified Redlich-Kister equation; (——), calculated values with NRTL model; (——), calculated values with UNIQUAC model. At T = 313.15 K: (△), experimental data; (----), calculated values with modified Redlich-Kister equation; (----), calculated values with NRTL model; (----), calculated values with UNIQUAC model.

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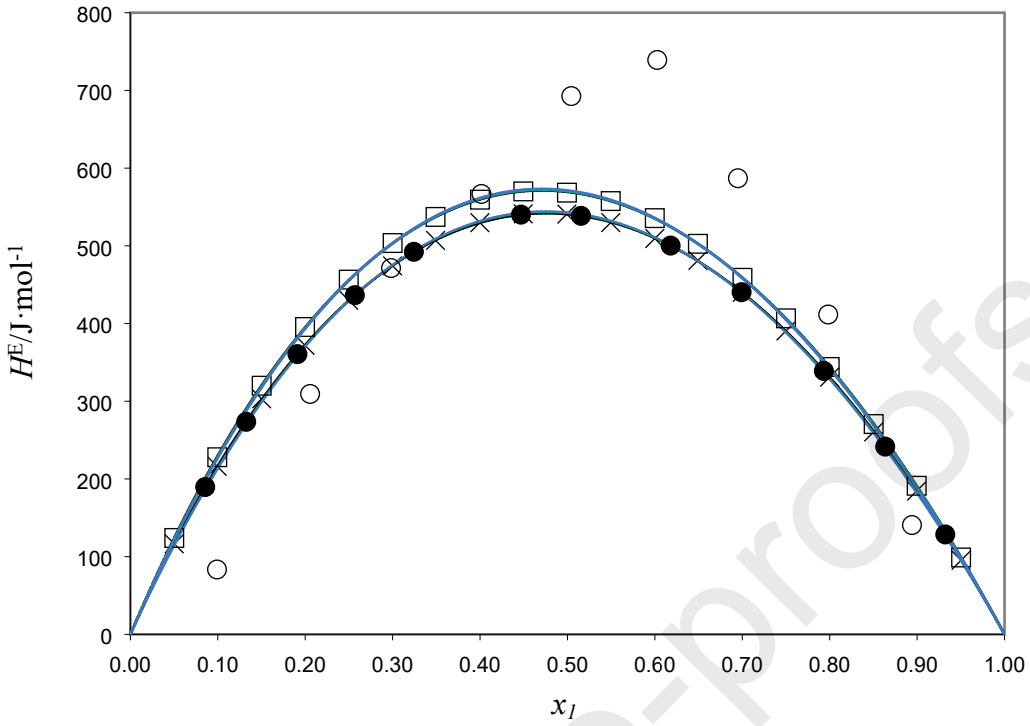
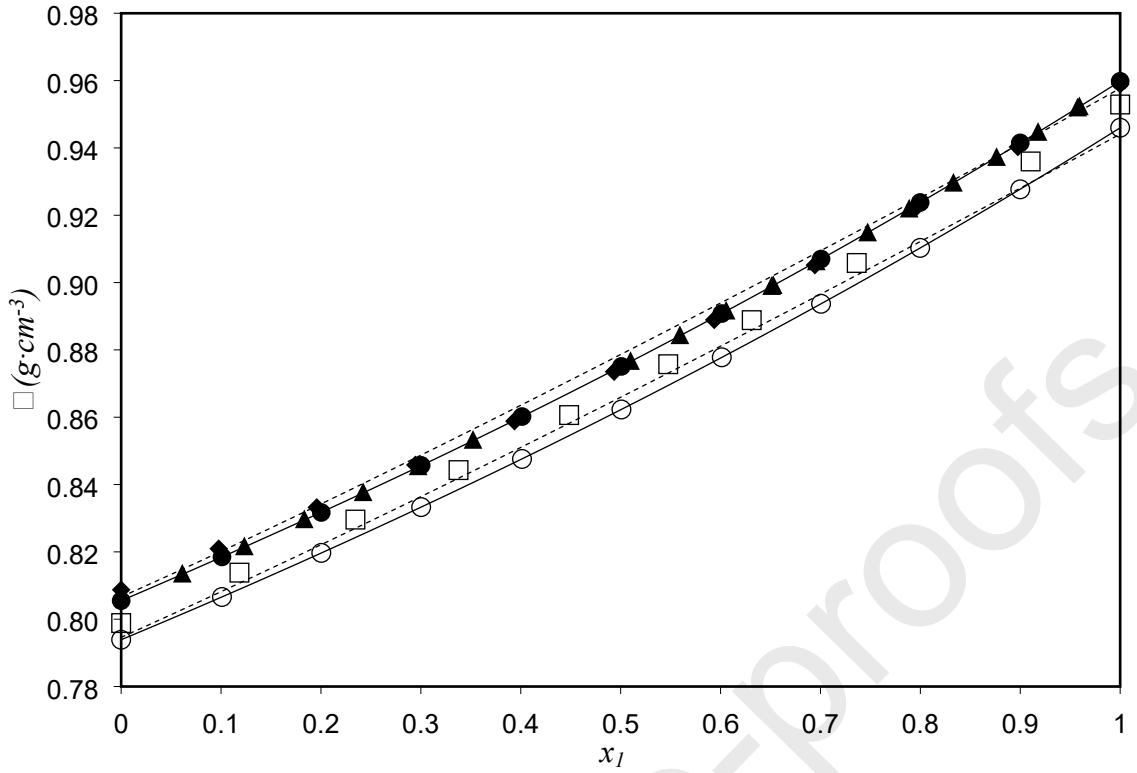


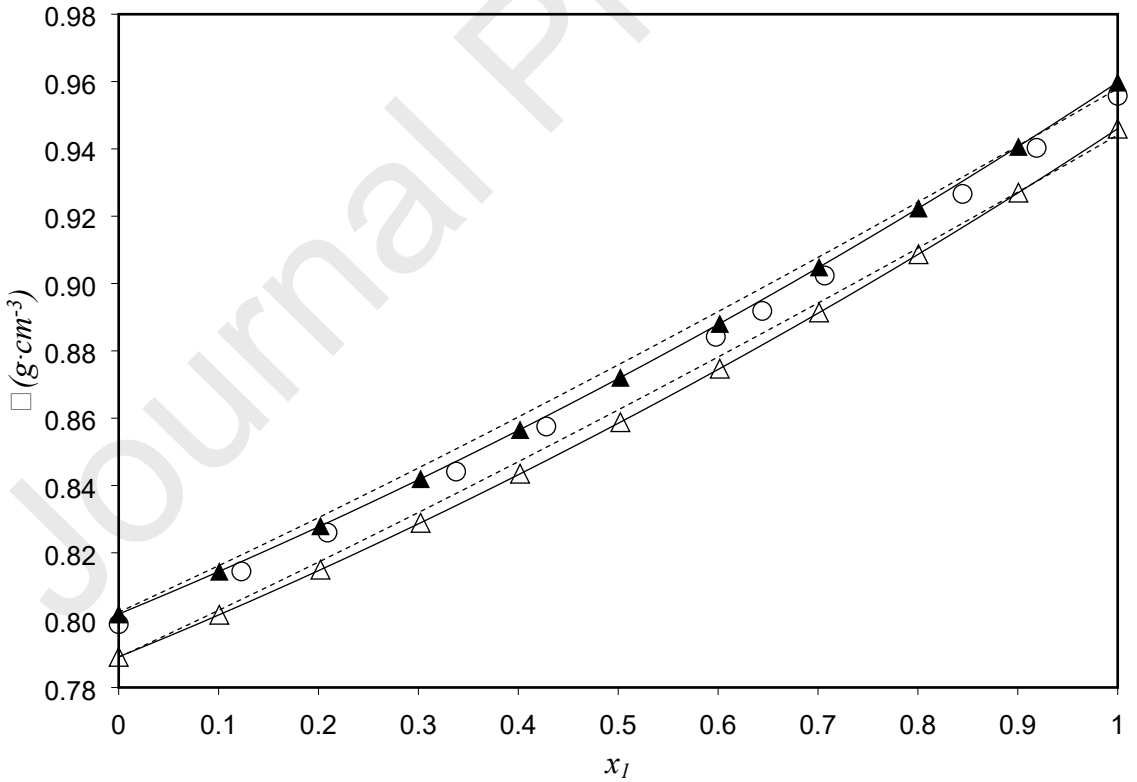
Figure 3. Excess enthalpy H^E of 2-methoxyethanol (1) + 1-propanol (2). At T = 298.15 K: (■), experimental data; (●), Reddy et *al.* [79]; (——), calculated values with modified Redlich-Kister equation; (——), calculated values with NRTL model; (——), calculated values with UNIQUAC model. At T = 313.15 K: (□), experimental data; (----), calculated values with modified Redlich-Kister equation; (----), calculated values with NRTL model; (----), calculated values with UNIQUAC model; (○), Chandak et *al.* [92] at 321.15 K.

(a)

Journal Pre-proofs



(b)



Journal Pre-proofs

(c)

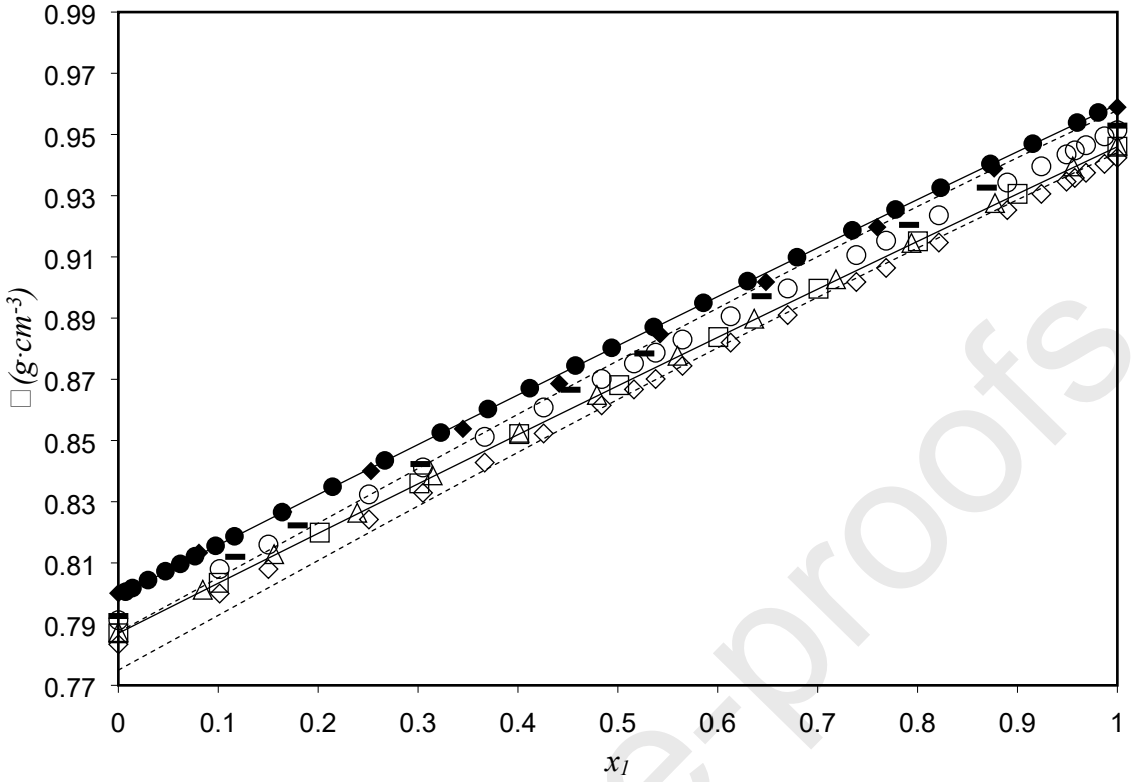
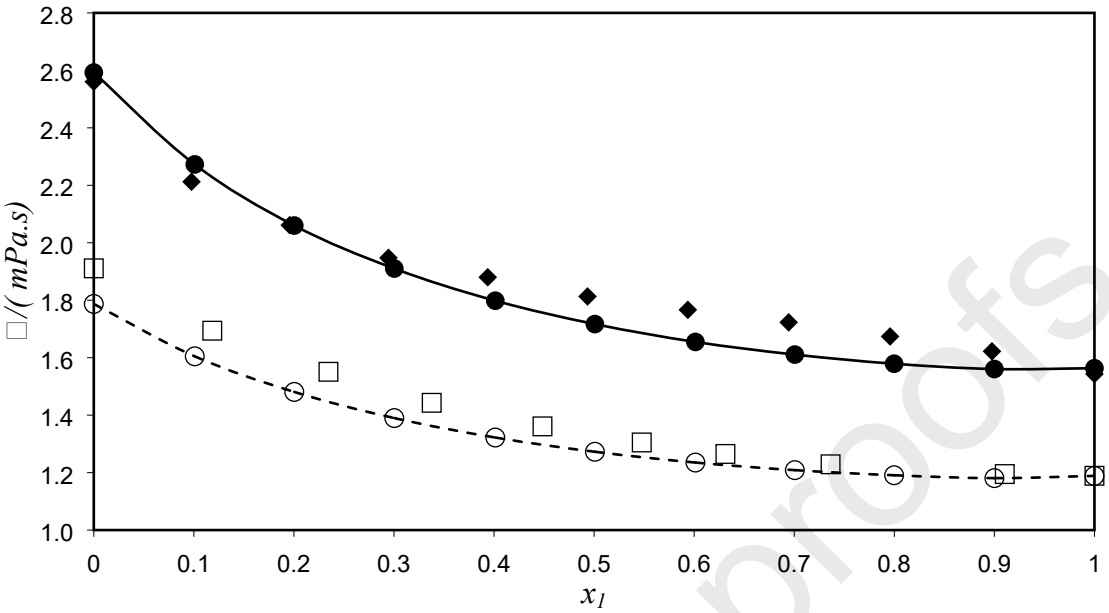


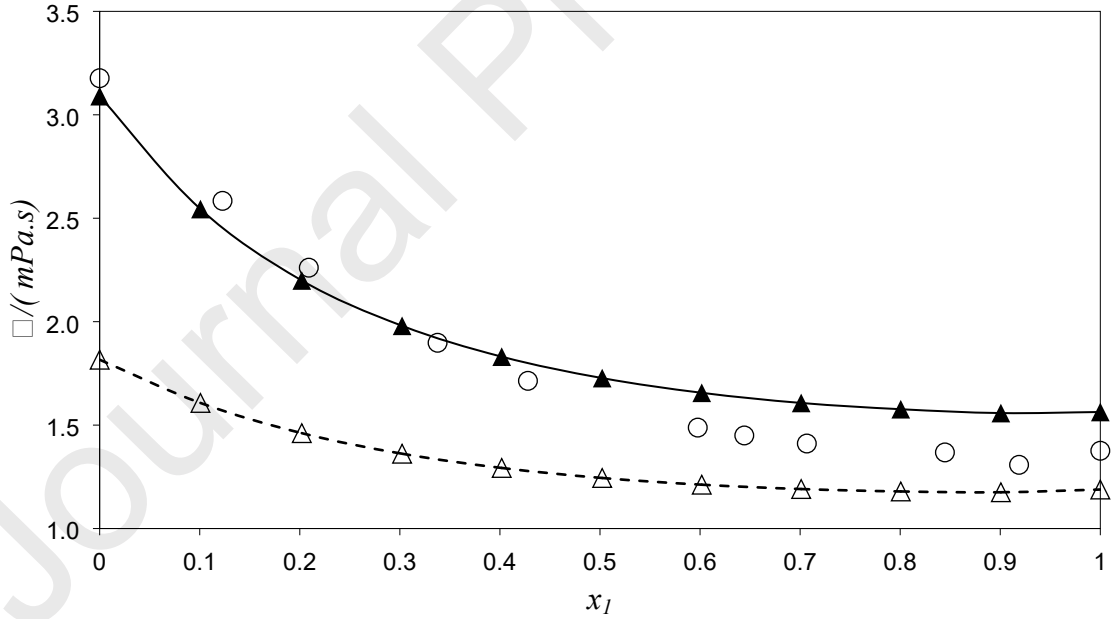
Figure 4. Experimental values of densities, ρ, as a function of mole fraction of x_1 for binary mixtures: (a), 2-methoxyethanol (1) + 1-butanol (2), (●), this work at 298.15 K, (♦), Roy et *al.* [81] at 298.15 K, (▲), Mozo et *al.* [83] at 298.15 K, Reddy et *al.* [94] at 308.15 K, (○), this work at 313.15 K, (□); (b), 2-methoxyethanol (1) + 2-butanol (2), (▲), this work at 298.15 K, (○), Krishnan et al. [95] at 303.15 K, (△), this work at 313.15 K; and (c), 2-methoxyethanol (1) + 1-propanol (2), (■), this work at 298.15 K, (♦), Roy et *al.* [81], (●), Pal et *al.* [90] at 298.15 K, (○), Pal et *al.* [93] at 308.15 K, (▬), Reddy et *al.* [94] at 308.15 K, (□), this work at 313.15 K, (△), Zarei et *al.* [82] at 313.15 K, (◊), Pal et *al.* [93] at 318.15 K. (——), calculated values of density with the polynomial equation (Eq. 11); (----), calculated values of density with PC-SAFT equation of state.

Journal Pre-proofs

(a)



(b)



Journal Pre-proofs

(c)

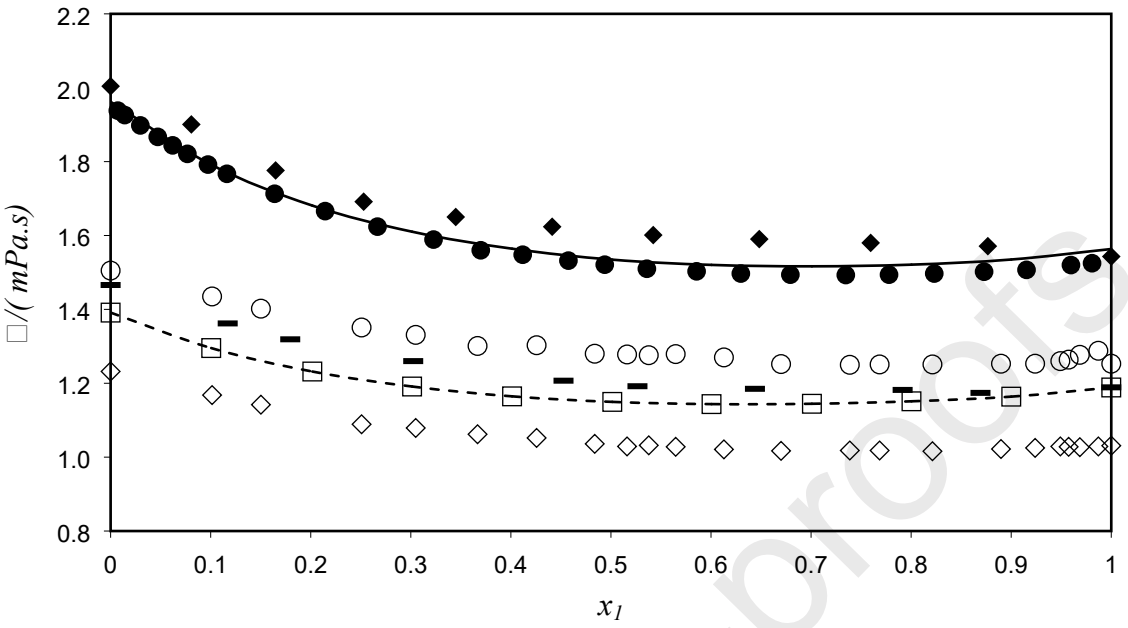
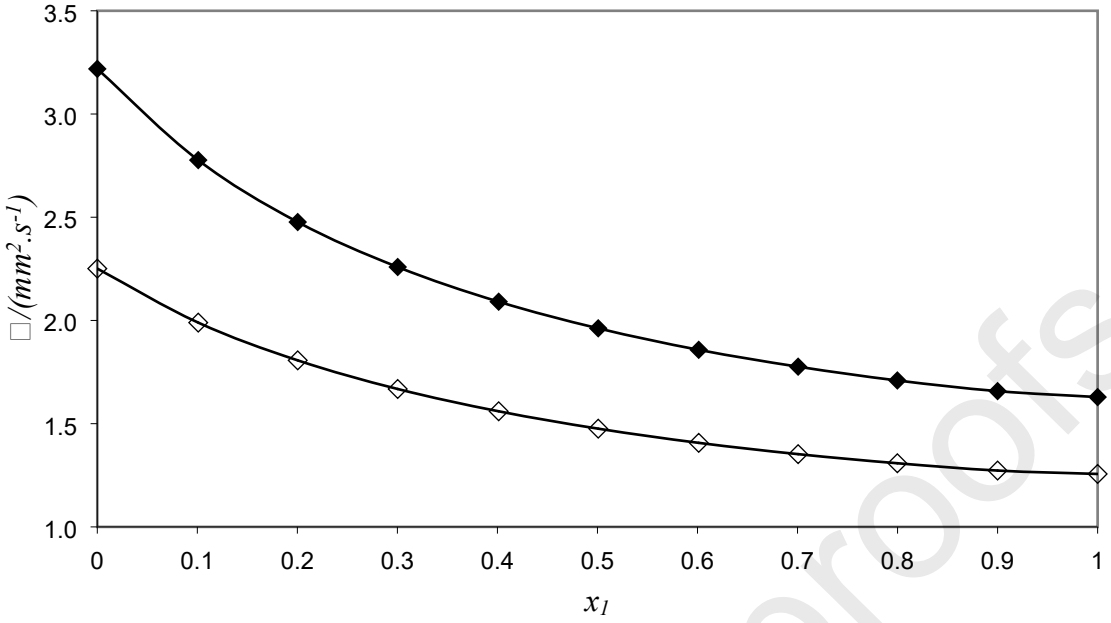


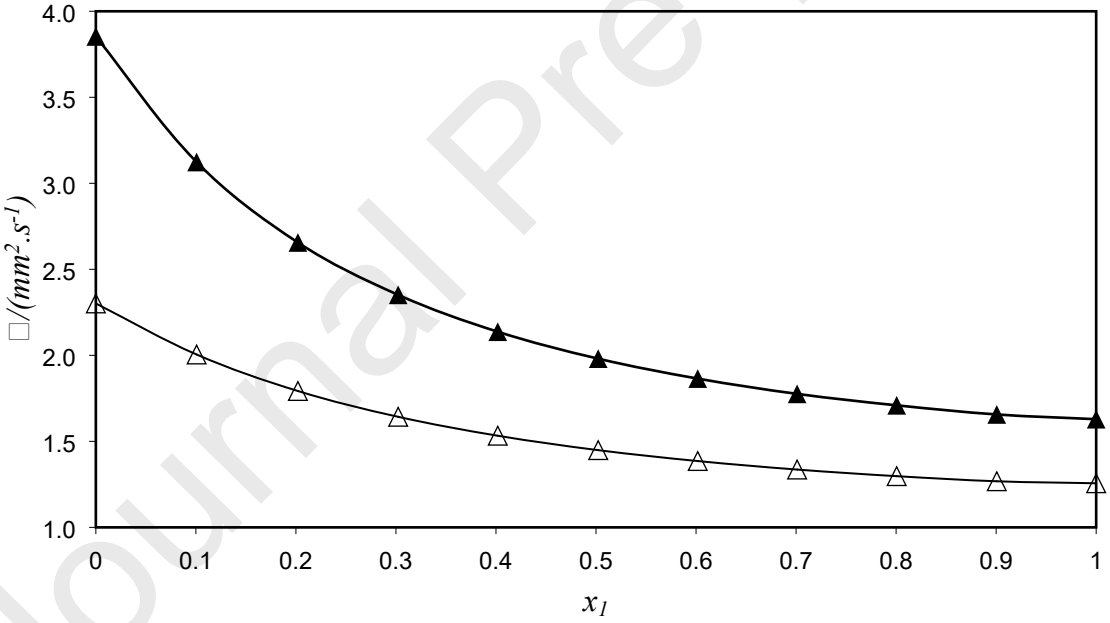
Figure 5. Experimental values of dynamic viscosity, η, as a function of mole fraction of x_1 for binary mixtures: (a), 2-methoxyethanol (1) + 1-butanol (2), (●), this work at 298.15 K, (♦), Roy et *al.* [81] at 298.15 K, (□), Reddy et *al.* [94] at 308.15 K, (○), this work at 313.15 K; (b), 2-methoxyethanol (1) + 2-butanol (2), (▲), this work at 298.15 K, (○), Krishnan et *al.* [95] at 303.15 K, (△), this work at 313.15 K; and (c), 2-methoxyethanol (1) + 1-propanol (2), (■), this work at 298.15 K, (♦), Roy et *al.* [81], (●), Pal et *al.* [90] at 298.15 K, (○), Pal et *al.* [93] at 308.15 K, (▬), Reddy et *al.* [94] at 308.15 K, (□), this work at 313.15 K, (◊), Pal et *al.* [93] at 318.15 K. (——), calculated values of dynamic viscosity with the polynomial equation (Eq. 11).

(a)

Journal Pre-proofs



(b)



(c)

Journal Pre-proofs

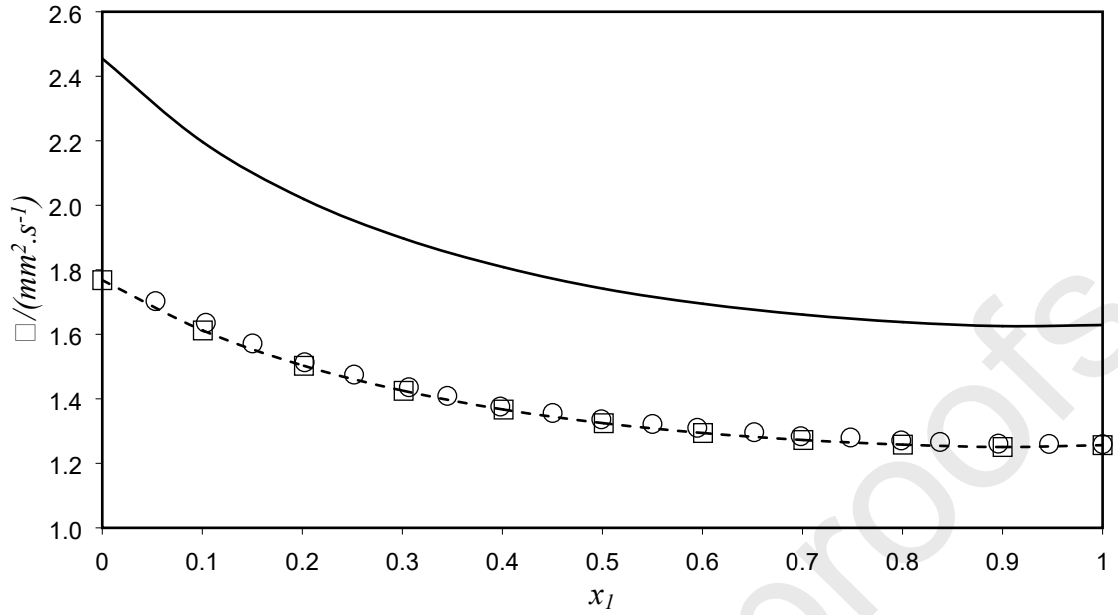
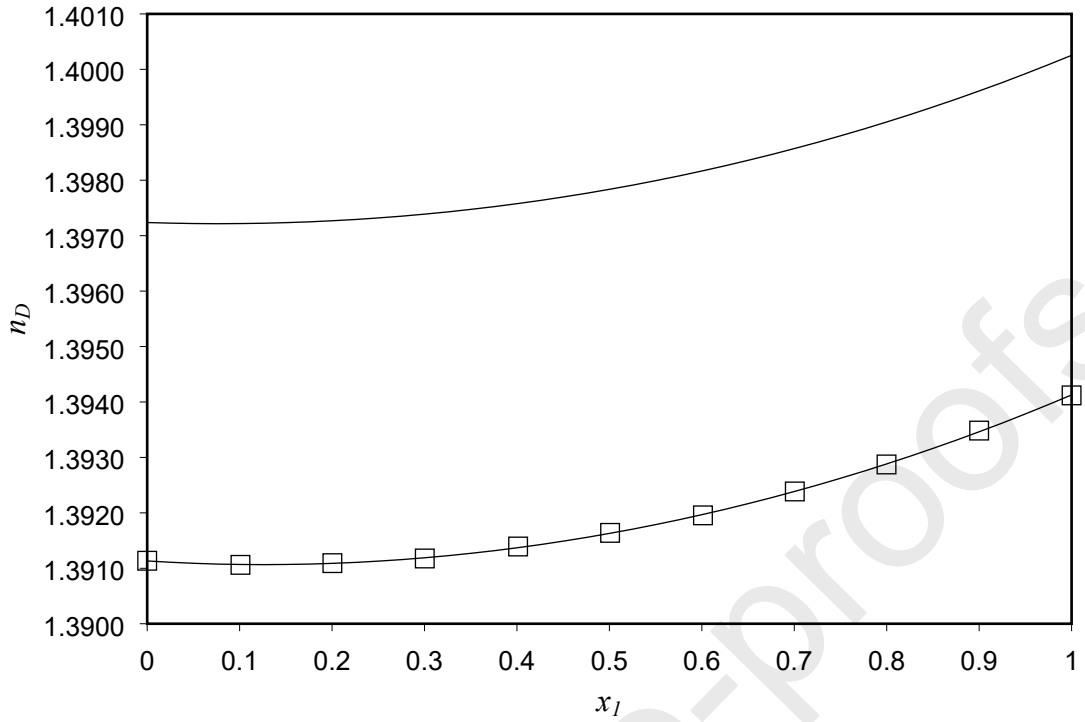


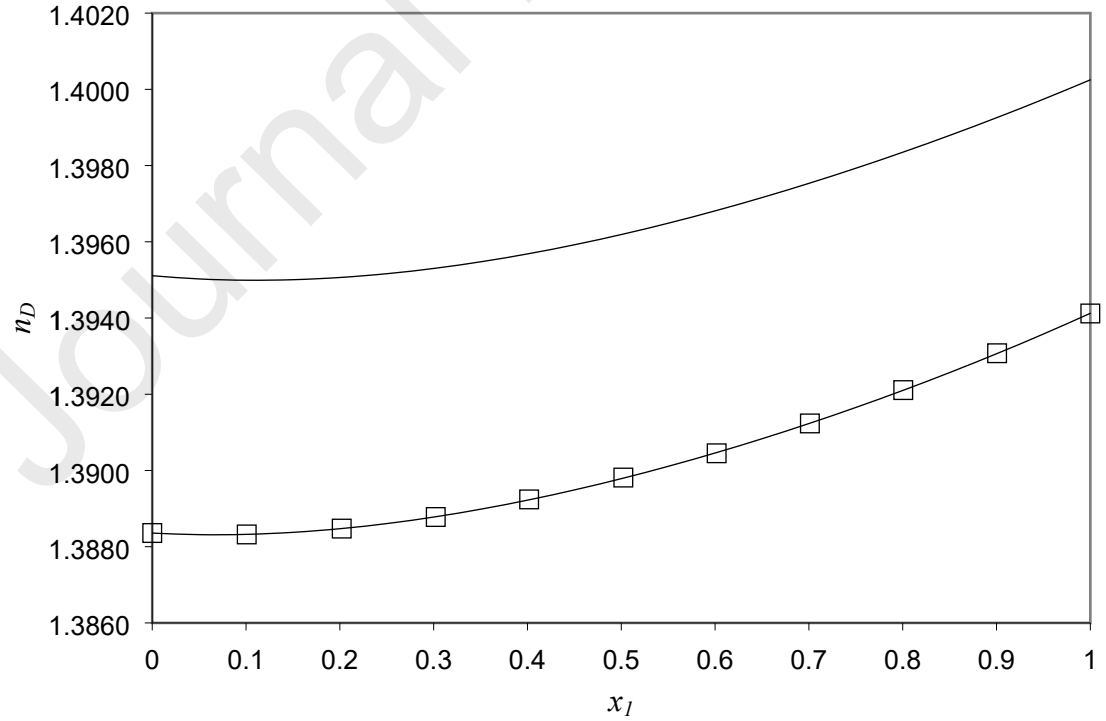
Figure 6. Experimental values of kinematic viscosity, υ, as a function of mole fraction of x_1 for binary mixtures: (a), 2-methoxyethanol (1) + 1-butanol (2), (♦), this work at 298.15 K, (◊), This work at 313.15 K. (b), 2-methoxyethanol (1) + 2-butanol (2), (▲), 298.15 K and (△). 313.15 K. And (c), 2-methoxyethanol (1) + 1-propanol (2), (■), this work at 298.15 K, (□), this work at 313.15 K, (○), Chandak et *al.* [92] at 313.15 K. (——), calculated values of kinematic viscosity with the polynomial equation (Eq. 11).

(a)

Journal Pre-proofs



(b)



Journal Pre-proofs

(c)

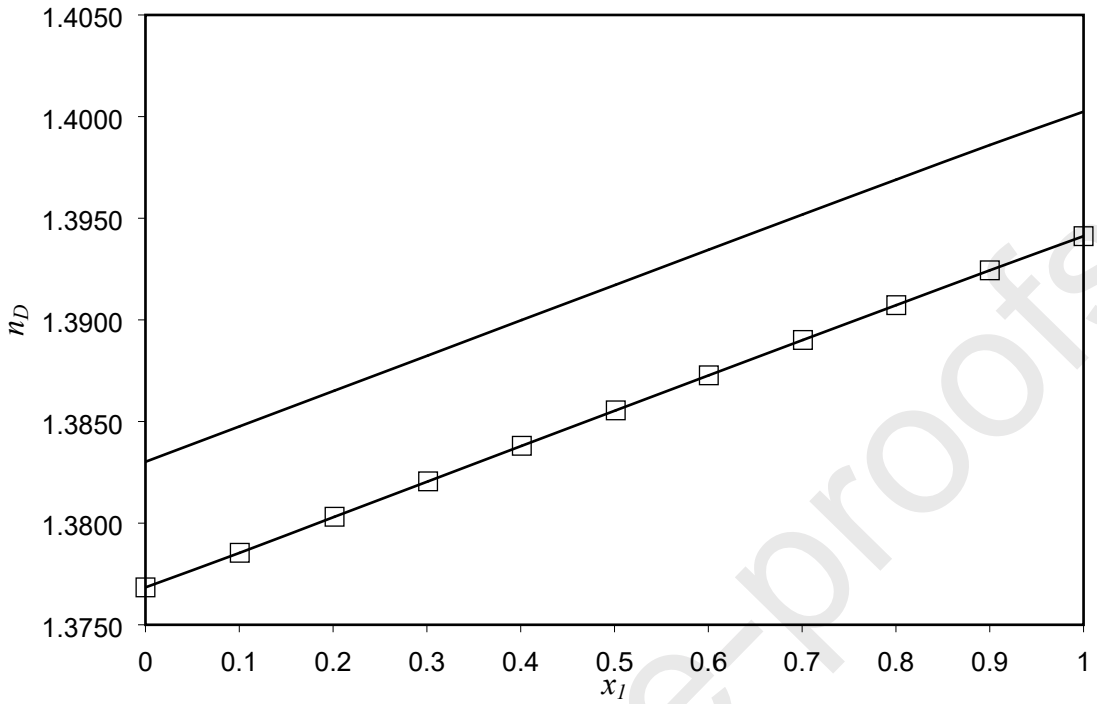
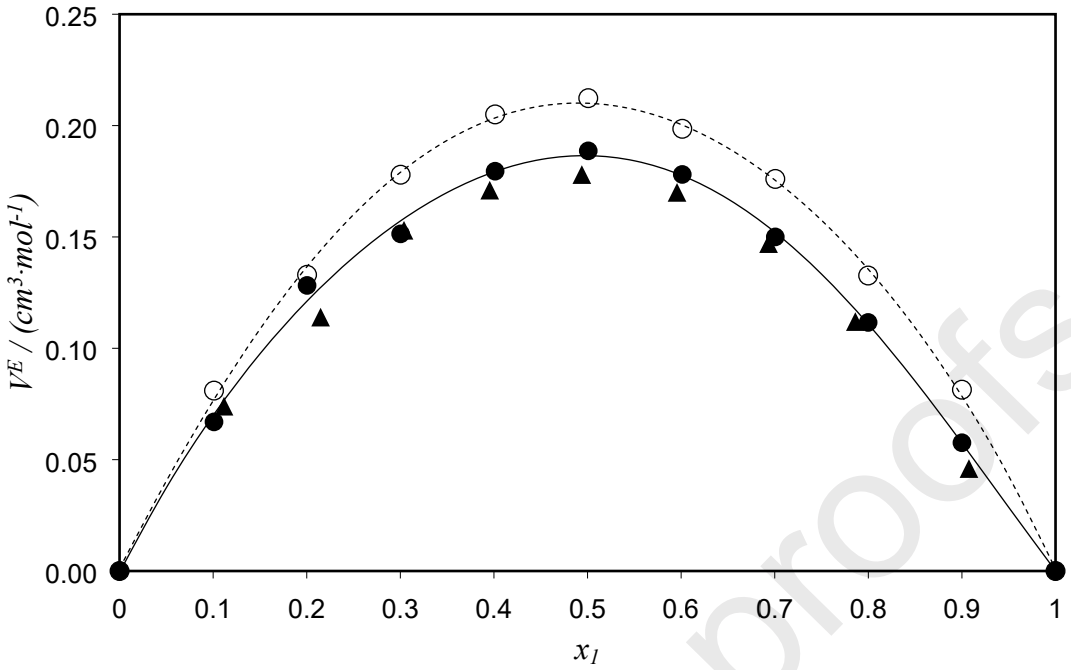


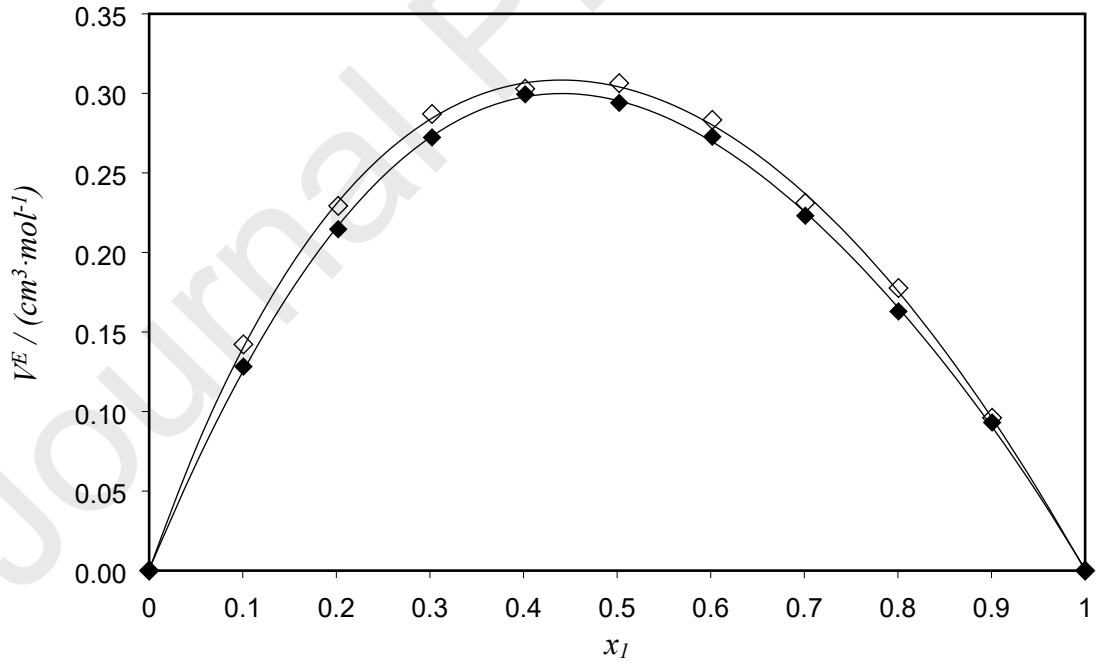
Figure 7. Experimental values of refractive index, n_D, as a function of mole fraction of x_1 for binary mixtures: (a), 2-methoxyethanol (1) + 1-butanol (2); (b), 2-methoxyethanol (1) + 2-butanol (2); and (c), 2-methoxyethanol (1) + 1-propanol (2). At temperatures: (■), 298.15 K and (□), 313.15 K. (——), calculated values of refractive index with the polynomial equation (Eq. 11).

(a)

Journal Pre-proofs



(b)



(c)

Journal Pre-proofs

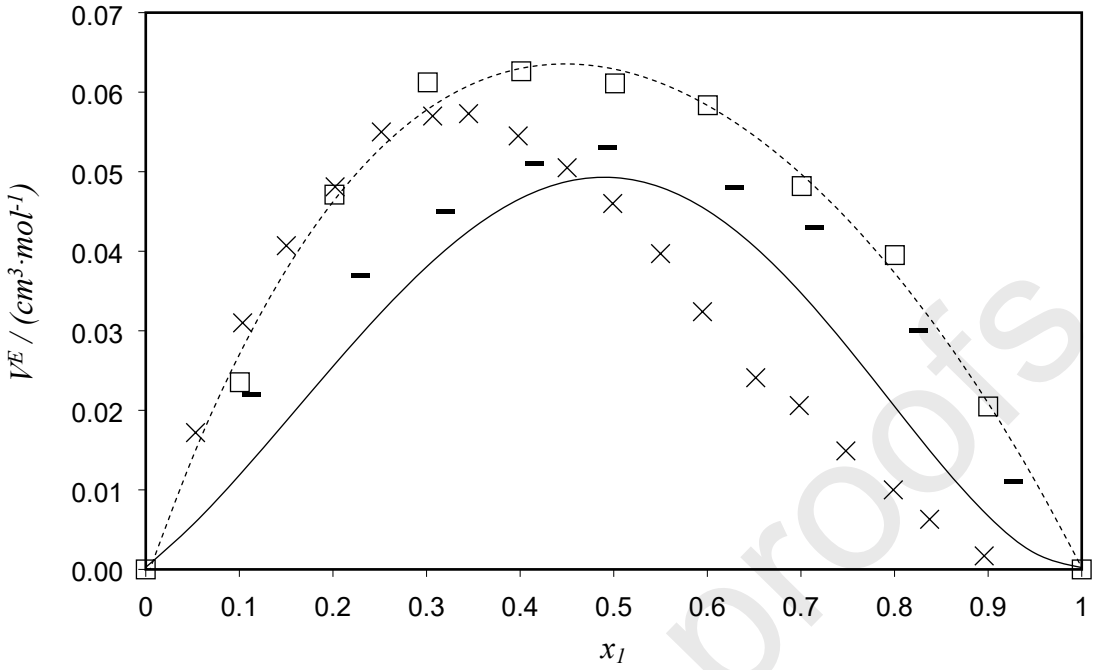
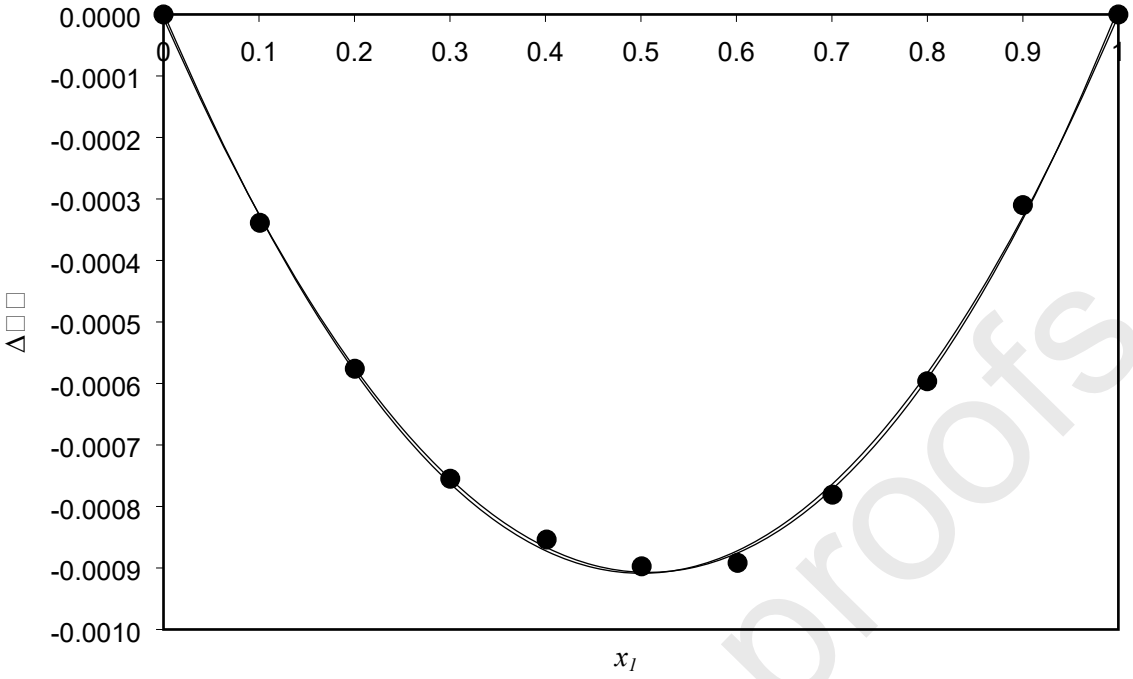


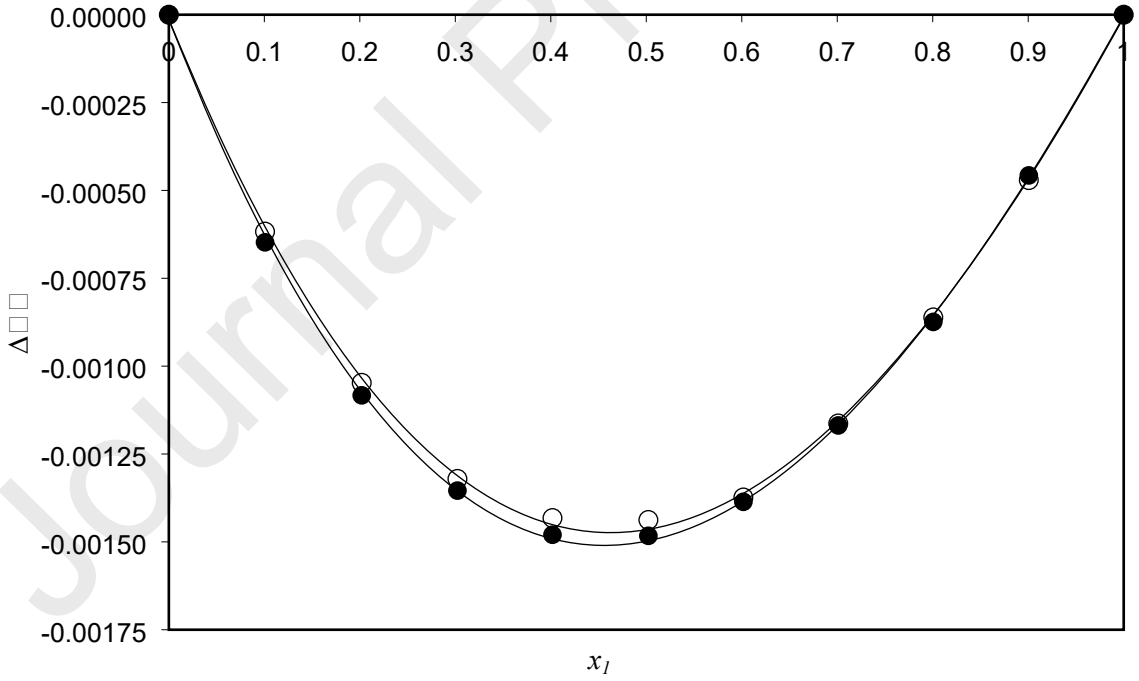
Figure 8. Calculated values of excess volume, V^E, as a function of mole fraction of x_1 for binary mixtures: (a), 2-methoxyethanol (1) + 1-butanol (2), (●), this work at 298.15 K, (▲), Cobos et *al.* [91] at 298.15 K, (○), this work at 313.15 K. (b), 2-methoxyethanol (1) + 2-butanol (2), (♦), this work at 298.15 K, (◊), this work at 313.15 K. And (c), 2-methoxyethanol (1) + 1-propanol (2). (■), this work at 298.15 K, (▬), Pal et *al.* [90] at 298.15 K, (□), this work at 313.15 K, (×), Chandak et *al.* [92] at 313.15 K. (——), calculated values of excess volume with the Redlich-Kister equation (Eq. 12) at 298.15 K.

(a)

Journal Pre-proofs



(b)



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(c)

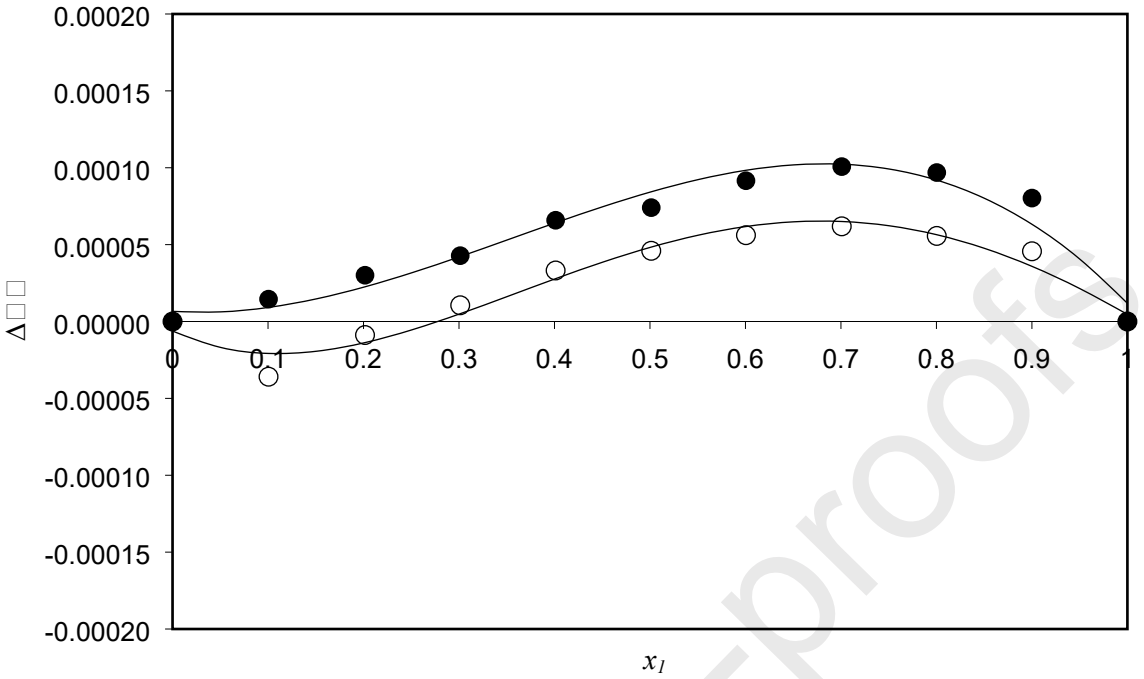


Figure 9. Calculated values of deviations in refractive index, Δn_D, as a function of mole fraction of x_1 for binary mixtures: (a), 2-methoxyethanol (1) + 1-butanol (2); (b), 2-methoxyethanol (1) + 2-butanol (2); and (c), 2-methoxyethanol (1) + 1-propanol (2). At temperatures: (●), 298.15 K and (○), 313.15 K. (——), calculated values of deviations in refractive index with the Redlich-Kister (Eq. 12) at 298.15 K.

Table 1. Purity and chemical data of used liquids.

Compound	Formula	Molar mass (g/mol)	State mole fraction purity (mol%)	CAS number
2-Methoxyethanol	$C_3H_8O_2$	76.09	>99.8[1]	109-86-4
1-Butanol	$C_4H_{10}O$	74.12	>99.8[1]	71-36-3

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2-Butanol*	$C_4H_{10}O$	74.12	>99.0[1]	78-92-2
1-Propanol	C_3H_8O	60.09	>99.7[1]	71-23-8

[1] Determined by gas chromatography (GC) by the supplier Sigma-Aldrich.

* Racemic mixture

Table 2. Comparison of measured data of density, ρ, dynamic viscosity, η, and refractive index n_D of the pure components (2-methoxyethanol, 1-butanol, 2-butanol and 1-propanol) with the corresponding literature data at (298.15 and 313.15) K and at 0.1 MPa.[a]

Component	T/(K)	ρ/(g/cm^3)		η/(mPa.s)		n_D	
		Exp	Lit	Exp	Lit	Exp	Lit
2-Methoxyethanol	298.15	0.9598	0.9601[18]	1.563	1.552[18]	1.4002	1.4001[31]
			0.9602[19]		1.542[19]		1.4002[32]

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			0.9602[21]		1.590[23]		1.4005[32]
			0.9602[22]		1.544[24]		1.4007[33]
			0.9602[23]		1.592[26]		1.4004[34]
			0.9602[24]		1.541[27]		
			0.9600[18]		1.512[28]		
			0.9602[25]		1.543[39]		
			0.9602[26]				
	313.15	0.9460	0.9459[20]	1.188	1.162[20]	1.3941	1.3942[35]
			0.9463[23]		1.180[23]		1.3941[37]
			0.9463[29]		1.189[40]		1.3930[38]
			0.9423[30]		1.173[41]		
			0.9462[35]				
			0.9462[36]				
			0.9459[38]				
1-Butanol	298.15	0.8055	0.8060[42]	2.593	2.619[42]	1.3972	1.3972[50]
			0.8059[43]		2.620[46]		1.3972[51]
			0.8057[44]		2.509[44]		1.3972[52]
			0.8057[45]		2.561[45]		1.3967[56]
			0.8060[49]		2.606[49]		1.3993[56]
			0.8057[50]		2.539[50]		1.3974[57]
			0.8056[51]				1.3973[58]
	313.15	0.7939	0.7933[42]	1.787	1.786[42]	1.3911	1.3908[56]
			0.7945[43]		1.754[46]		1.3920[57]
			0.7941[44]		1.706[44]		1.3935[65]
			0.7943[45]		1.681[47]		1.3910[65]

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			0.7943[47]		1.795[61]		1.3910[68]
			0.7943[49]				
			0.7944[61]				
2-Butanol	298.15	0.8018	0.8025[50]	3.090	3.093[50]	1.3951	1.3952[50]
			0.8026[51]		3.132[53]		1.3950[51]
			0.8025[58]		3.068[54]		1.3950[52]
			0.8025[58]		2.998[55]		1.3951[58]
			0.8025[59]		2.954[63]		1.3953[58]
			0.8025[63]		3.068[64]		1.3953[63]
			0.8020[54]		2.998[64]		1.3951[68]
			0.8020[64]				
	313.15	0.7891	0.7922[60]	1.816	1.801[60]	1.3884	1.3885[63]
			0.7896[61]		1.840[61]		1.3883[65]
			0.7895[61]		1.785[61]		1.3860[65]
			0.7907[62]		1.782[62]		1.3890[68]
			0.7896[63]		1.766[63]		1.3881[68]
			0.7895[65]				
			0.7894[65]				
1-Propanol	298.15	0.7991	0.7994[42]	1.961	1.981[42]	1.3830	1.3832[56]
			0.7995[43]		1.970[46]		1.3837[56]
			0.7996[44]		1.898[44]		1.3838[57]
			0.7996[49]				1.3836[58]
			0.7996[58]				1.3837[58]
			0.7996[58]				1.3830[68]

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			0.7997[59]				
	313.15	0.7870	0.7866[42]	1.391	1.381[42]	1.3768	1.3774[56]
			0.7873[43]		1.361[46]		1.3785[57]
			0.7875[44]		1.319[44]		1.3770[68]
			0.7870[48]		1.378[48]		1.3775[68]
			0.7874[49]		1.379[66]		1.3770[68]
			0.7885[66]		1.379[67]		
			0.7873[67]				

[a] Expanded uncertainties u are $u(T)$ = 0.04 K, $u(p)$ = 0.001 MPa and the combined expanded uncertainties Uc in density, dynamic viscosity and refractive index are $Uc(\rho)$ = 0.0005 g.cm^{-3}, $Uc(\eta)$ = 0.02η and $Uc(n_D)$ = 0.005, respectively, (0.95 level of confidence).

Table 3. Sets of parameters A_i, with standard deviations σ, needed for correlation of density, ρ, dynamic viscosity, η, kinematic viscosity, υ, and refractive index, n_D, by employing the polynomial equation (Eq. 11) for the studied binary mixtures at (298.15 and 313.15) K and at 0.1 MPa.[a]

	T (K)	A_1	A_2	A_3	A_4	σ
	x_1 2-methoxyethanol (1) + (1- x_1) 1-butanol (2) [*]					
ρ	298.15	0.80550	0.12620	0.02319	0.00494	$1.3\cdot10^{-8}$
	313.15	0.79388	0.12409	0.02215	0.00585	$9.2\cdot10^{-9}$
η	298.15	2.5261	-2.3607	1.4343	-	$1.3\cdot10^{-2}$
	313.15	1.7530	-1.4016	0.8549	-	$3.6\cdot10^{-3}$
υ	298.15	3.1290	-3.2835	1.8343	-	$2.5\cdot10^{-2}$
	313.15	2.2036	-2.0244	1.1036	-	$7.0\cdot10^{-3}$

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n_D	298.15	1.3972	-0.0005	0.0032	0.0003	$1.5 \cdot 10^{-9}$
	313.15	1.3911	-0.0010	0.0039	0.0001	$1.7 \cdot 10^{-9}$
	x_1 2-methoxyethanol (1) + (1- x_1) 2-butanol (2) [*]					
ρ	298.15	0.80179	0.12294	0.03275	0.00229	$6.7 \cdot 10^{-9}$
	313.15	0.78905	0.12186	0.03264	0.00241	$2.1 \cdot 10^{-8}$
η	298.15	2.9526	-3.6868	2.3772	-	$5.9 \cdot 10^{-2}$
	313.15	1.7731	-1.5836	1.0245	-	$6.1 \cdot 10^{-3}$
υ	298.15	3.6723	-4.9511	3.0139	-	$1.0 \cdot 10^{-1}$
	313.15	2.2421	-2.2588	1.3094	-	$1.2 \cdot 10^{-2}$
n_D	298.15	1.3951	-0.0018	0.0091	-0.0021	$1.4 \cdot 10^{-9}$
	313.15	1.3883	-0.0009	0.0084	-0.0017	$2.1 \cdot 10^{-9}$
	x_1 2-methoxyethanol (1) + (1- x_1) 1-propanol (2) [*]					
ρ	298.15	0.79914	0.16702	-0.00644	0.00013	$2.2 \cdot 10^{-8}$
	313.15	0.78701	0.16426	-0.00492	-0.00036	$5.0 \cdot 10^{-9}$
η	298.15	1.9242	-1.2443	0.9044	-	$4.4 \cdot 10^{-3}$
	313.15	1.3716	-0.7302	0.5573	-	$1.2 \cdot 10^{-3}$
υ	298.15	2.4013	-1.9326	1.1911	-	$9.0 \cdot 10^{-3}$
	313.15	1.7386	-1.2108	0.7450	-	$2.7 \cdot 10^{-3}$
n_D	298.15	1.3830	0.0170	0.0012	-0.0010	$1.2 \cdot 10^{-9}$
	313.15	1.3768	0.0171	0.0009	-0.0007	$7.1 \cdot 10^{-10}$

[a] Expanded uncertainties u are $u(T)$ = 0.04 K, $u(p)$ = 0.001 MPa and the combined expanded uncertainties Uc in mole fraction, density, dynamic viscosity, kinematic viscosity and refractive index are $U\text{c}(x)$ = 0.0005, $U\text{c}(\rho)$ = 0.0005 g.cm^{-3}, $U\text{c}(\eta) = 0.02\eta$, $U\text{c}(\upsilon) = 0.02\upsilon$ and $U\text{c}(n_D)$ = 0.005, respectively, (0.95 level of confidence).

[*] x_1: mole fraction of component 1 (2-methoxyethanol).

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Table 4. Sets of parameters A_i, with standard deviations σ, using for correlation of excess volume, V^E, and deviations in refractive index, Δn_D, by employing the Redlich-Kister equation for the studied binary mixtures at (298.15 and 313.15) K and at 0.1 MPa.[a]

	T (K)	A_1	A_2	A_3	σ
	x_1 2-methoxyethanol (1) + (1- x_1) 1-butanol (2) [*]				
V^E	298.15	0.74610	-0.04975	-0.06025	$1.3\cdot10^{-4}$
	313.15	0.83979	-0.00791	0.03001	$7.2\cdot10^{-5}$
Δn_D	298.15	-0.00363	-0.00009	-0.00004	$1.6\cdot10^{-9}$
	313.15	-0.00399	0.00002	-0.00003	$1.7\cdot10^{-9}$
	x_1 2-methoxyethanol (1) + (1- x_1) 2-butanol (2) [*]				
V^E	298.15	1.18189	-0.26269	0.02475	$5.8\cdot10^{-5}$
	313.15	1.21726	-0.28396	0.14504	$9.0\cdot10^{-5}$
Δn_D	298.15	-0.00595	0.00109	-0.00034	$6.1\cdot10^{-10}$
	313.15	-0.00581	0.00089	-0.00040	$9.3\cdot10^{-10}$
	x_1 2-methoxyethanol (1) + (1- x_1) 1-propanol (2) [*]				
V^E	298.15	0.19698	-0.02517	-0.14728	$1.1\cdot10^{-5}$
	313.15	0.25187	-0.04615	0.02395	$4.0\cdot10^{-5}$
Δn_D	298.15	0.00030	0.00036	0.00031	$1.9\cdot10^{-10}$
	313.15	0.00019	0.00037	-0.00017	$5.9\cdot10^{-10}$

[*] x_1: mole fraction of component 1 (2-methoxyethanol).

Table 5. Characteristic Parameters of PC-SAFT model for 2-methoxyethanol, 1-butanol, 2-butanol and 1-propanol.

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Compound	m [–]	**σ** [A]	**ε**/*k* [K]	ε^{HB}/k [**K**]	K^{HB} *[K]*	AAD % (ρ^{Liq})
2-Methoxyethanol	2.98978	3.28153	212.809	0.1518400	2245.71	0.014
1-Butanol	4.38072	3.04936	218.502	0.0402697	2246.18	0.030
2-Butanol	3.68544	3.21794	213.009	0.0312056	2085.52	0.040
1-Propanol	2.99974	3.25221	233.402	0.0152681	2276.84	0.006

Table 6. Experimental data of H^E of studied mixtures x_1 2-methoxyethanol (1) + (1- x_1) 1-butanol (2), x_1 2-methoxyethanol (1) + (1- x_1) 2-butanol (2) and x_1 2-methoxyethanol (1) + (1- x_1) 1-propanol (2) at (298.15 and 313.15) K and at 0.1 MPa.[a]

x	H^E/J·mol^{-1}	x	H^E/J·mol^{-1}	x	H^E/J·mol^{-1}	x	H^E/J·mol^{-1}
x_1 2-methoxyethanol (1) + (1- x_1) 1-butanol (2) *							
298.15 K							
0.0494	123.7	0.3003	538.1	0.5499	629.6	0.8004	412.0
0.0997	237.5	0.3502	580.4	0.6004	610.8	0.8499	329.9
0.1494	334.4	0.3994	609.1	0.6502	579.8	0.8999	233.2
0.1999	416.6	0.4494	627.0	0.6992	537.5	0.9503	121.5
0.2497	483.9	0.5000	633.7	0.7502	480.3		
313.15 K							
0.0494	143.7	0.3003	609.2	0.5498	694.1	0.8003	441.2
0.0997	271.1	0.3501	654.5	0.6003	669.7	0.8498	351.9
0.1493	381.0	0.3994	683.1	0.6500	632.0	0.8998	247.3
0.1999	474.7	0.4492	700.1	0.6991	582.5	0.9503	128.7
0.2497	550.1	0.4999	704.2	0.7501	517.1		
x_1 2-methoxyethanol (1) + (1- x_1) 2-butanol (2) *							

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			298.15 K				
0.0496	174.1	0.2997	727.0	0.5495	809.3	0.7999	504.0
0.1001	333.2	0.3497	776.0	0.6000	777.4	0.8504	398.4
0.1500	465.1	0.4004	808.2	0.6498	731.3	0.9003	279.2
0.2006	573.8	0.4504	822.7	0.7002	669.3	0.9505	144.7
0.2505	660.6	0.4996	822.5	0.7497	592.6		
			313.15 K				
0.0496	153.7	0.2996	674.0	0.5494	757.5	0.7998	470.8
0.1001	296.2	0.3496	722.2	0.5998	727.7	0.8504	372.7
0.1499	418.3	0.4004	753.4	0.6497	682.8	0.9002	260.2
0.2006	523.8	0.4503	768.4	0.7000	626.5	0.9505	135.7
0.2505	608.5	0.4995	771.0	0.7496	555.8		
			x_1 2-methoxyethanol (1) + (1- x_1) 1-propanol (2) *				
			298.15 K				
0.0502	116.5	0.3000	474.2	0.5495	529.9	0.7999	331.0
0.0993	216.2	0.3491	507.0	0.5999	509.4	0.8503	260.5
0.1501	303.1	0.3998	529.8	0.6492	481.2	0.8994	184.4
0.1998	371.9	0.4494	541.2	0.7000	440.2	0.9503	95.3
0.2498	429.9	0.4993	540.8	0.7499	390.4		
			313.15 K				
0.0502	124.0	0.2999	503.6	0.5493	557.6	0.7999	344.1
0.0993	228.0	0.3490	537.2	0.5998	535.7	0.8503	270.7
0.1501	320.0	0.3997	559.4	0.6490	502.6	0.8994	191.3
0.1997	395.6	0.4493	570.1	0.7000	458.9	0.9503	99.0
0.2497	456.5	0.4993	568.5	0.7498	406.7		

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[a] Expanded uncertainties of pressure p, temperature T and mole fraction x are as follows: $u(p)$= 0.001 MPa, $u(T)$ = 0.05 K, $u(x)$ = 0.0005. The relative expanded uncertainty (k = 2) is $U_r(H^E)$ = 0.01 for excess enthalpy.

[*] x_1: mole fraction of component 1 (2-methoxyethanol).

Table 7. Sets of parameters needed for the graphical representation of excess enthalpies H^E by modified Redlich-Kister equation (Eq. 1) for studied mixtures x_1 2-methoxyethanol (1) + (1- x_1) 1-butanol (2), x_1 2-methoxyethanol (1) + (1- x_1) 2-butanol (2) and x_1 2-methoxyethanol (1) + (1- x_1) 1-propanol (2) at (298.15 and 313.15) K.[*]

Binary Systems			
298.15 K	*2ME (1) + 1-But (2)[a]*	*2ME (1) + 2-But (2)[a]*	*2ME (1) + 1-Pro (2)[a]*
A_o	0.3255	0.1932	0.4266
A_1	2538.4	3296.1	2162.9
A_2	823.7	296.5	719.8
A_3	121.5	101.8	-
AAD (%)	0.3%	0.3%	0.2%
rms ΔH^E/J·mol^{-1}	1.2	1.5	0.6
Max $\lvert\Delta H^E\rvert$/J·mol^{-1}	1.6	2.0	0.9
Max ($\lvert\Delta H^E\rvert/H^E$)	1.8%	2.0%	0.6%
313.15 K	*2ME (1) + 1-But (2)[a]*	*2ME (1) + 2-But (2)[a]*	*2ME (1) + 1-Pro (2)[a]*
A_o	0.5609	0.1172	0.3230
A_1	2819.4	3086.2	2277.7
A_2	1429.2	94.7	477.9
AAD (%)	0.3%	0.4%	0.1%
rms ΔH^E/J·mol^{-1}	1.4	2.1	0.6
Max $\lvert\Delta H^E\rvert$/J·mol^{-1}	2.0	3.0	1.0
Max ($\lvert\Delta H^E\rvert/H^E$)	1.2%	2.9%	0.4%

[a] *2ME: 2-Methoxyethanol; 1-But: 1-Butanol; 2-But: 2-Butanol; 1-Pro: -Propanol.*
[*] x_1: mole fraction of component 1 (2-methoxyethanol).

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Table 8. Sets of parameters needed for the graphical representation of excess molar enthalpies H^E by NRTL and UNIQUAC models, for studied binary mixtures x_1 2-methoxyethanol (1) + (1- x_1) 1-butanol (2), x_1 2-methoxyethanol (1) + (1- x_1) 2-butanol (2) and x_1 2-methoxyethanol (1) + (1- x_1) 1-propanol (2) at (298.15 and 313.15) K.*

Binary Systems[a]				
2ME (1) + 1-But (2)[b]	NRTL		UNIQUAC	
	298.15 K	***313.15 K***	***298.15 K***	***313.15 K***
A_0	0.6214	0.5804	633.3	678.4
A_1	0.6452	0.7868	-36.0	-49.9
α_{12}	0.30	0.30	-	-
AAD (%)	0.5%	0.2%	1.1%	0.8%
rms ΔH^E/J·mol^{-1}	2.5	1.1	4.9	3.9
Max $\lvert\Delta H^E\rvert$/J·mol^{-1}	4.6	2.1	7.9	5.5
Max ($\lvert\Delta H^E\rvert/H^E$)	1.4%	0.8%	2.9%	2.2%
2ME (1) + 2-But (2)[b]	NRTL		UNIQUAC	
	298.15 K	***313.15 K***	***298.15 K***	***313.15 K***
A_0	0.7417	0.6240	457.1	634.4
A_1	1.1133	0.9242	279.7	34.7
α_{12}	0.30	0.30	-	-
AAD (%)	0.6%	1.0%	0.7%	0.4%
rms ΔH^E/J·mol^{-1}	2.1	3.8	4.5	1.7
Max $\lvert\Delta H^E\rvert$/J·mol^{-1}	3.7	8.7	7.1	3.0
Max ($\lvert\Delta H^E\rvert/H^E$)	3.3%	5.5%	1.7%	2.8%
2ME (1) + 1-Pro (2)[b]	NRTL		UNIQUAC	
	298.15 K	***313.15 K***	***298.15 K***	***313.15 K***
A_0	0.3599	0.3377	342.6	461.4
A_1	0.6992	0.7318	129.2	20.4
α_{12}	0.30	0.30	-	-

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AAD (%)	0.4%	0.2%	0.8%	0.6%
rms ΔH^E/J·mol^{-1}	1.7	1.0	2.7	2.0
Max $\lvert\Delta H^E\rvert$/J·mol^{-1}	3.4	1.8	4.7	2.9
Max ($\lvert\Delta H^E\rvert/H^E$)	1.5%	0.9%	2.1%	1.7%

[a] *Equivalence between parameters: NRTL $A_0=\tau_{12}$ and $A_1=\tau_{21}$; UNIQUAC $A_0=\Delta u_{12}$; $A_1=\Delta u_{21}$.*

[b] *2ME: 2-Methoxyethanol; 1-But: 1-Butanol; 2-But: 2-Butanol; 1-Pro: 1-Propanol.*

[*] x_1: mole fraction of component 1 (2-methoxyethanol).

Table 9. Experimental density, ρ, dynamic viscosity, η, kinematic viscosity, υ, and refractive index, n_D, for the binary mixtures x_1 2-methoxyethanol (1) + (1- x_1) 1-butanol (2), x_1 2-methoxyethanol (1) + (1- x_1) 2-butanol (2) and x_1 2-methoxyethanol (1) + (1- x_1) 1-propanol (2) at (298.15 and 313.15) K and at 0.1 MPa.[a]

x_1	ρ/(g/cm^3)	η/(mPa.s)	υ/(mm^2.s^{-1})	n_D
x_1 2-methoxyethanol (1) + (1- x_1) 1-butanol (2) [*]				
T = 298.15 K				
0.1009	0.8185	2.27	2.78	1.3972
0.2003	0.8317	2.06	2.48	1.3973
0.3003	0.8457	1.91	2.26	1.3974
0.4012	0.8602	1.80	2.09	1.3976
0.5008	0.8751	1.72	1.96	1.3978
0.6012	0.8908	1.65	1.86	1.3982
0.7006	0.9070	1.61	1.78	1.3986
0.7998	0.9238	1.58	1.71	1.3990
0.9000	0.9415	1.56	1.66	1.3996
T = 313.15 K				
0.1009	0.8066	1.60	1.99	1.3911
0.2003	0.8197	1.48	1.81	1.3911

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0.3003	0.8333	1.39	1.67	1.3912
0.4012	0.8476	1.32	1.56	1.3914
0.5008	0.8623	1.27	1.48	1.3916
0.6012	0.8778	1.24	1.41	1.3920
0.7006	0.8937	1.21	1.35	1.3924
0.7998	0.9103	1.19	1.31	1.3929
0.9000	0.9277	1.18	1.27	1.3935

x_1 2-methoxyethanol (1) + (1- x_1) 2-butanol (2) *

T = 298.15 K

0.1007	0.8145	2.54	3.12	1.3950
0.2020	0.8280	2.20	2.66	1.3951
0.3022	0.8420	1.98	2.35	1.3953
0.4018	0.8566	1.83	2.14	1.3957
0.5022	0.8721	1.73	1.98	1.3962
0.6017	0.8881	1.66	1.86	1.3968
0.7010	0.9049	1.61	1.78	1.3975
0.8006	0.9224	1.58	1.71	1.3983
0.9006	0.9407	1.56	1.66	1.3993

T = 313.15 K

0.1007	0.8016	1.61	2.00	1.3883
0.2020	0.8150	1.46	1.79	1.3885
0.3022	0.8289	1.36	1.64	1.3888
0.4018	0.8435	1.29	1.53	1.3892
0.5022	0.8588	1.24	1.45	1.3898
0.6017	0.8747	1.21	1.39	1.3905

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0.7010	0.8914	1.19	1.34	1.3912
0.8006	0.9087	1.18	1.30	1.3921
0.9006	0.9270	1.18	1.27	1.3931

x_1 2-methoxyethanol (1) + (1- x_1) 1-propanol (2) *

T = 298.15 K

0.1005	0.8159	1.79	2.20	1.3848
0.2016	0.8326	1.68	2.02	1.3865
0.3013	0.8489	1.61	1.90	1.3883
0.4012	0.8651	1.56	1.81	1.3900
0.5013	0.8812	1.53	1.74	1.3917
0.6005	0.8971	1.52	1.69	1.3935
0.7008	0.9131	1.52	1.66	1.3952
0.8003	0.9288	1.52	1.64	1.3969
0.9001	0.9444	1.54	1.63	1.3986

T = 313.15 K

0.1005	0.8035	1.30	1.61	1.3785
0.2016	0.8199	1.23	1.50	1.3803
0.3013	0.8360	1.19	1.42	1.3821
0.4012	0.8521	1.16	1.37	1.3838
0.5013	0.8681	1.15	1.32	1.3855
0.6005	0.8838	1.14	1.29	1.3873
0.7008	0.8996	1.14	1.27	1.3890
0.8003	0.9151	1.15	1.26	1.3907
0.9001	0.9306	1.16	1.25	1.3924

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[a] Expanded uncertainties u are $u(T)$ = 0.04 K, $u(p)$ = 0.001 MPa and the combined expanded uncertainties Uc in mole fraction, density, dynamic viscosity, kinematic viscosity and refractive index are $Uc(x)$ = 0.0005, $Uc(\rho)$ = 0.0005 g.cm^{-3}, $Uc(\eta)$ = 0.02η, $Uc(\upsilon)$ = 0.02υ and $Uc(n_D)$ = 0.005, respectively, (0.95 level of confidence).

[*] x_1: mole fraction of component 1 (2-methoxyethanol).

- New data of H^E, ρ, η, υ, and n_D for binary mixtures are reported.
- Derived properties were calculated.
- Redlich-Kister equation, NRTL and UNIQUAC models were used.
- PC-SAFT EoS was applied in this work.
- Intermolecular effects involved in these systems have been discussed

CRediT author statement

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