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Density, Viscosity, Refractive Index, and Related Thermophysical Properties of Dibutyl Ether +2-Butanol + Cyclohexane Ternary Systems

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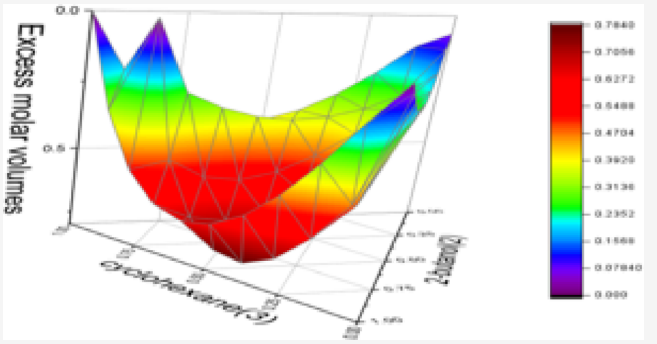
ABSTRACT: New measured data for density, (ρ), dynamic and kinematic viscosities, (μ_D and μ_c), and refractive index, (n_D), are presented at T = 298.15 K and p = 0.1 MPa for binary and ternary mixtures containing dibutyl ether, 2-butanol, and cyclohexane. As a result, the derived properties are estimated based on the measured data. Excess molar volume, (V^E), dynamic viscosity deviation ($\Delta\mu_D$), and deviation in refractive index, (Δn_D), as derived properties, are fitted using the Redlich−Kister equation. In addition, perturbed-chain statistical associating fluid theory equation of state is employed to correlate the measured data of density.



1. INTRODUCTION

For the industrial and transportation sectors, fossil fuels such as coal, oil, and natural gas are the primary sources of energy. Fossil fuels, which are considered non-renewable energy sources, account for more than 80% of the world's primary energy supply.[1] The global demand for energy is steadily increasing owing primarily to population increase and economic development. If the current consumption rates continue, oil and gas reserves will be consumed completely by the end of the century.[2,3] Additionally, transportation is a significant consumer of fossil fuels. Petroleum-based liquid fuels, such as gasoline, diesel, liquefied petroleum gas, and natural gas, are commonly used in automobiles.[4] These non-renewable materials contribute to environmental damage and climate change. In this context, a transition to alternate energy sources is urgently required in order to lessen the toxicity of pollutants released by automobiles. Previous research has shown that biofuels, which are generated directly from plants, are the best renewable alternative to fossil fuels. In Brazil, Australia, India, United States of America, and European Union, the majority of gasoline is blended with biofuels like ethanol and bio-ethers. In the same lines, the use of ethers and alcohols as oxygenated gasoline additives yields positive results due to their capacity to reduce pollutants and enhance the octane number.[5] Some oxygenated components were added to the gasoline reformulation, such as alcohols, ethers, and glycol ethers, in order to increase the octane rating and lower the toxicity of the contaminants.[6] Our research into the thermophysical characteristics of binary and ternary mixtures containing oxygenated components with alcohols and hydrocarbon components[7−17] led to this paper. At 0.1 MPa and 298.15 K, a study of density, dynamic and kinematic viscosities, and refractive index for binary mixtures composed of (i) dibutyl ether (1) + 2-butanol (2), (ii) dibutyl ether (1) + cyclohexane (2), (iii) 2-butanol (1) + cyclohexane (2), and the ternary mixture constituted by dibutyl ether (1) + 2-butanol (2) + cyclohexane (3) is presented in this work. The following derived properties are calculated using reported measured data: V^E, $\Delta\mu_D$, and Δn_D. The Redlich−Kister equation is employed to fit the derived properties. Furthermore, the varied observed densities for studied binary and ternary mixtures are modeled using the perturbed-chain statistical associating fluid theory equation of state (PC-SAFT EoS). The influence of intermolecular interactions is examined in this paper for all binary and ternary mixtures studied.

2. EXPERIMENTAL SECTION

2.1. Apparatus and Procedure. At 0.1 MPa and 298.15 K, a Stabinger SVM 3000 viscosimeter is used to measure

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densities (ρ), and dynamic and kinematic viscosities (μ_D and μ_c), for pure components (dibutyl ether, 2-butanol, and cyclohexane) as well as for binary and ternary mixtures. Two rotating concentric tubes make up this apparatus. Its working mode is based on the Couette principle, which asserts that viscosity is proportional to torque difference between rotating cylinders. The relative uncertainty of μ_D is 2% (k = 2), μ_c is 3% (k = 2), and the expanded uncertainties of ρ, T, p, and x_i are 0.0005 g.cm^{-3} (k = 2, level of confidence: 95.45%), 0.04 K, 0.01 MPa, and 0.0008, respectively. The refractive index (n_D) of the pure components, as well as their binary and ternary mixtures, is measured using an Abbe digital refractometer. The refractive index has an expanded uncertainty of 0.00005 (k = 2, 0.95 degree of confidence). Air and decane are used to calibrate the Stabinger SVM 3000 viscosimeter, while air and water are used to calibrate the Abbe digital refractometer.

2.2. Chemicals. Dibutyl ether (DBE), 2-butanol, and cyclohexane are the chemicals used in this work, and they are given with a high mole fraction purity (>99%). Table 1 lists the chemical characteristics of the investigated components. Using an OHAUS analytical balance with a precision of 0.0001 g, different mixtures composed of dibutyl ether, 2-butanol, and cyclohexane are created by mass. The mole fraction standard uncertainty is predicted to be 0.0008. Table 2 compares the pure component's experimental density, dynamic viscosity, and refractive index to data previously published in the literature.[18−59]

Table 1. Purity and Related Data of Chemicals

compound	formula	molar ass (g·mol^{-1})	state mole fraction purity[a]	CAS number
2-butanol	$C_4H_{10}O$	74.12	0.990	78-92-2
dibutyl ether	$C_8H_{18}O$	130.23	0.993	142-96-1
cyclohexane	C_6H_{12}	84.20	0.999	110-82-7

[a]Determined by gas chromatography by the supplier Sigma Aldrich.

3. MODELING

Gross and Sadowski developed the PC-SAFT EoS,[60,61] which can be written, in terms of the residual Helmholtz energy ($\breve{a}^{res}$), as the sum of a hard-chain energy contribution ($\breve{a}^{hc}$), a dispersive energy contribution($\breve{a}^{disp}$), and an association interaction energy ($\breve{a}^{assoc}$)

$$\breve{a}^{res} = \breve{a}^{hc} + \breve{a}^{disp} + \breve{a}^{assoc} \tag{1}$$

The non-associative parameters of the PC-SAFT EoS are segment number (m), segment energy parameter (ε/k), and segment diameter (σ). However, for complex fluids like associative fluids, it is advisable to include two additional parameters: the association volume (k^{A_iBi}) and the association energy (ε^{A_iBi}).

The Berthelot−Lorentz conventional mixing rule describes the parameters σ_{ij} and ε_{ij} for the mixture:

$$\sigma_{ij} = \left(\frac{\sigma_{ii} + \sigma_{jj}}{2}\right) \tag{2}$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_{ii}\varepsilon_{jj}}\,(1 - k_{ij}) \tag{3}$$

where k_{ij} is the binary interaction parameter for correcting the interaction between unequal chains segments. The binary interaction parameters are assumed to be zero for the mixtures analyzed in this study.

The PC-SAFT equation of state parameters are optimized using the following objective function:

$$Obj.\ F = \sum_{i=1}^{N}\left(\frac{\rho_i^{exp} - \rho_i^{calc}}{\rho_i^{exp}}\right)^2 \tag{4}$$

nwhere N is the number of measured data.

PC-SAFT EoS parameters were generated by fitting the measured density of studied pure components in this work. Due to the good representation of density of all studied mixtures, two associating sites (2B association scheme) were used.

The PC-SAFT EoS takes the size and shape of the molecules into account and is based on statistical mechanics.[62−64] Furthermore, the association is explicitly taken into account in the PC-SAFT EoS, which is crucial for modeling the mixtures discussed in this paper.

4. CORRELATION OF DENSITY, VISCOSITY, REFRACTIVE INDEX, AND DERIVED PROPERTIES

4.1. Binary and Ternary Mixtures. A mathematical polynomial equation is used to fit the density, ρ, for binary mixtures:

$$P = \sum_{i=0}^{N} A_i \times x_1^{\,i-1} \tag{5}$$

where the P function presented ρ, x_1 is the mole fraction of component 1, and A_i coefficients are calculated using the unweighted least-squares approach, and the optimal number of A_i is established using the F-test.[65]

The calculation of dynamic viscosity is done according to ref 66 written as

$$\mu_D = x_1 \times \mu_{D1} + (1 - x_1) \times \mu_{D2} + x_1(1 - x_1) \times \left\{\sum_{i=0}^{2} C_i \cdot (1 - 5x_1)^i\right\} \tag{6}$$

with x_1: the mole fraction of component 1; C_i: the adjustment coefficients; μ_{D1} and μ_{D2}: dynamic viscosity of pure components of each binary mixture.

The excess molar volumes for all mixtures over a wide range of mole fractions are calculated using the equation:

$$V^E = \sum_{i=1}^{n} x_i M_i\left[\left(\frac{1}{\rho}\right) - \left(\frac{1}{\rho_i}\right)\right] \tag{7}$$

where n is the number of pure components in the mixture, x_i denotes the mole fraction of component i, and M_i is the molar mass, while the measured densities of the pure component i and the mixture are ρ_i and ρ, respectively.

From the experimental values of viscosity for binary and ternary mixtures and corresponding mole fractions, dynamic viscosity deviation ($\Delta\mu_D$), are calculated using the following equation:

$$\Delta\mu_D = \mu_D - \sum_{i=1}^{n} x_i\mu_{D_i} \tag{8}$$

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J. Chem. Eng. Data XXXX, XXX, XXX−XXX

Table 2. Comparison of Experimental Density, ρ, Dynamic Viscosity, μ_D, and Refractive Indices, n_D, of the Pure Component with the Corresponding Literature Values at T = 298.15 K and at p = 0.1 MPa[a]

	ρ (g/cm^3)		μ_D (mPa·s)		n_D	
component	exp	lit	exp	lit	exp	lit
dibutyl ether	0.7630	0.7641[18]	0.66	0.64[26]	1.39651	1.39887[18]
		0.7641[22]		0.65[27]		1.39650[29]
		0.7638[23]		0.64[21]		1.39650[18]
		0.7639[24]		0.64[29]		1.39680[26]
		0.7641[24]				1.39640[19]
		0.7641[25]				1.39660[27]
2-butanol	0.8015	0.8023[30]	3.13	3.10[35]	1.39511	1.39540[37]
		0.8025[37]		3.07[34]		1.39523[31]
		0.8027[31]		3.09[32]		1.39480[38]
		0.8027[38]		3.07[46]		1.39540[47]
		0.8024[39]				1.39503[32]
		0.8023[40]				1.39510[48]
		0.8022[41]				1.39520[46]
		0.8024[42]				1.39530[33]
		0.8021[43]				
		0.8024[44]				
		0.8025[45]				
		0.8027[58]				
cyclohexane	0.7729	0.7732[53]	0.91	0.89[20]	1.42349	1.42350[53]
		0.7735[54]				1.42320[54]
		0.7739[57]				1.49840[36]
		0.7740[56]				1.42320[36]
		0.7739[55]				1.42310[50]
		0.7690[52]				1.42330[49]
		0.7692[51]				
		0.7739[28]				
		0.7739[50]				
		0.7691[59]				
		0.7739[58]				

[a]Standard uncertainties u are $u(T)$ = 0.04 K and u(p) = 0.01 MPa, and the combined expanded uncertainties U in density, dynamic viscosity, kinematic viscosity, and refractive index are $U(\rho)$ = 0.0005 g·cm^{-3}, $U(\mu_D)$ = 0.02 μ_D, $U(\mu_c)$ = 0.03 μ_c, and $U(n_D)$ = 0.00005, respectively (0.95 level of confidence).

where μ_{Di} is the absolute viscosity of pure component i and μ_D: is the absolute viscosity of the mixture.

The refractive index deviation, Δn_D, are calculated using the following equation:

$$\Delta n_D = n_D - \sum_{i=1}^{n} x_i n_{Di} \tag{9}$$

where n_D and n_{Di} represent the refractive index of the mixture and pure component i, respectively.

The following Redlich−Kister equation[66] is used to link derived properties such as V^E, $\Delta\mu_D$, and Δn_D:

$$\Delta Q = x_1 \times x_2 \sum_{i=0}^{N} D_i.\ (x_1 - x_2)^{i-1} \tag{10}$$

ΔQ functions could be excess molar volume, (V^E), dynamic viscosity deviation, $(\Delta\mu_D)$, or deviations in the refractive index, (Δn_D), x is the mole fraction, and D_i coefficients are generated using the unweighted least-squares method. The root-mean-square deviations σ are expressed as follows:

$$\sigma(X) = \left[\sum_{i=1}^{M} \frac{(X_{exp} - X_{calc})^2}{(n-p)}\right]^{1/2} \tag{11}$$

where X could be the density, (ρ), dynamic and kinematic viscosities, $(\mu_D$ and $\mu_c)$, or refractive index, (n_D); n: is the number of measured data, and$p$ is the parameter number used in the Redlich−Kister equation.

4.2. Ternary Mixtures. A mathematical polynomial equation is used to fit ρ for ternary mixtures:

$$H = \sum_{i=1}^{n} \sum_{j=1}^{M} B_{ij} \times x_i^j \tag{12}$$

where the H function presented ρ, B_{ij} coefficients are found using the unweighted least-squares approach, x_i is the mole fraction of the i coefficient, n is the component number, and M is the polynomial degree.

The following equation is used to fit excess molar volumes, (V^E), dynamic viscosity deviations, $(\Delta\mu_D)$, and deviations in the refractive index, (Δn_D), of ternary mixtures:

$$Y_{123} = Y_{12} + Y_{13} + Y_{23} + \Delta_{123} \tag{13}$$

where Y_{123} refers to V^E, $\Delta\mu_D$, or Δn_D of ternary mixtures. Y_{12}, Y_{13}, and Y_{23} refer to the corresponding contribution of three binary effect $(i + j)$: DBE (1) + 2-butanol (2), 2-butanol (1) + cyclohexane (2), and DBE (1) + cyclohexane (2) to the whole values of V^E, $\Delta\mu_D$, or Δn_D that are obtained by eq 10. Δ_{123}

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J. Chem. Eng. Data XXXX, XXX, XXX−XXX

refers to the contribution of ternary effect, which is described with the Cibulka typical semi-empirical equation:[74]

$$\Delta_{123} = F_0 + F_1 x_1 + F_2 x_2. \quad (14)$$

with x_i is the mole fraction.

Coefficients F_i and the corresponding standard deviations (σ) are generated using the least-squares method.

5. RESULTS AND DISCUSSION

5.1. Thermophysical Properties of Binary Mixtures. To compare the measured values of density with those derived with the assumed correlation, the absolute average deviation (AAD) is used in this work:

Table 3. Density, ρ, Dynamic Viscosity, μ_D, Kinematic Viscosity, μ_c, and Refractive Index, n_D, for the Binary Mixtures: DBE (1) + 2-Butanol (2), DBE (1) + Cyclohexane (2) and 2-Butanol (1) + Cyclohexane (2), at T = 298.15 K and at p = 0.1 MPa[a]

x_1	ρ (g·cm^{-3})	μ_D(mPa·s)	μ_c(mm^2·s^{-1})	n_D
		x_1 DBE + (1 − x_1) 2-Butanol		
0.0000	0.8015	3.13	3.91	1.39511
0.1005	0.7947	2.04	2.56	1.39521
0.2020	0.7888	1.49	1.88	1.39525
0.3015	0.7838	1.19	1.51	1.39529
0.4024	0.7794	1.00	1.28	1.39534
0.5023	0.7756	0.88	1.13	1.39542
0.5996	0.7724	0.80	1.04	1.39556
0.7021	0.7695	0.74	0.96	1.39574
0.8002	0.7670	0.70	0.92	1.39591
0.8984	0.7648	0.67	0.88	1.39615
1.0000	0.7630	0.66	0.86	1.39651
		x_1 DBE + (1 − x_1) Cyclohexane		
0.0000	0.7729	0.91	1.18	1.42349
0.1002	0.7700	0.83	1.08	1.41854
0.1969	0.7681	0.78	1.02	1.41480
0.2999	0.7666	0.74	0.97	1.41117
0.3978	0.7654	0.72	0.94	1.40819
0.4799	0.7648	0.70	0.92	1.40618
0.5992	0.7641	0.69	0.90	1.40339
0.6990	0.7636	0.68	0.89	1.40147
0.8002	0.7633	0.67	0.87	1.39962
0.9013	0.7631	0.66	0.87	1.39796
1.0000	0.7630	0.66	0.86	1.39651
		x_1 2-Butanol + (1 − x_1) Cyclohexane		
0.0000	0.7729	0.91	1.18	1.42343
0.0977	0.7729	0.89	1.16	1.41971
0.1976	0.7741	0.91	1.18	1.41616
0.2982	0.7758	0.95	1.23	1.41332
0.4011	0.7783	1.04	1.34	1.41018
0.4969	0.7810	1.14	1.46	1.40774
0.5997	0.7847	1.34	1.75	1.40448
0.6978	0.7881	1.56	1.98	1.40193
0.7997	0.7922	1.91	2.41	1.39942
0.9006	0.7971	2.44	3.06	1.39741
1.0000	0.8015	3.13	3.91	1.39517

[a]Standard uncertainties u are $u(T)$ = 0.04 K and $u(p)$ = 0.01 MPa, and the combined expanded uncertainties U in density, dynamic viscosity, kinematic viscosity, and refractive index are $U(\rho)$ = 0.0005 g·cm^{-3}, $U(\mu_D)$ = 0.02 μ_D, $U(\mu_c)$ = 0.03 μ_c, and $U(n_D)$ = 0.00005, respectively (0.95 level of confidence).

Table 4. Coefficients Needed for Eqs 5 and 6 with Standard Deviations Obtained for the Studied Binary Mixtures in this Work at T = 298.15 K and at p = 0.1 MPa

	DBE + 2-butanol	DBE + cyclohexane	2-butanol + cyclohexane
A_0	0.8015	0.7723	0.7728
A_1	−0.0657	−0.0222	−0.0012
A_2	0.0277	0.0132	0.0413
σ	0.008	0.007	0.003
C_0	1.7768	0.9643	1.3604
C_1	0.0260	−0.0264	−0.0090
C_2	0.0066	0.0294	0.0192
C_3	−0.0104	−0.0013	−0.0429
σ	0.04	0.03	0.07

Table 5. Coefficients D_i Needed for the Redlich−Kister Eq 10 with Standard Deviations Obtained for the Studied Binary Mixtures in This Work at T = 298.15 K and at p = 0.1 MPa

ΔQ	D_0	D_1	D_2	D_3	σ
		DBE + 2-Butanol			
V^E(cm^3·mol^{-1})	0.5558	0.2142	0.0495	0.3002	0.09
$\Delta\mu_D$ (mPa·s)	−4.0056	2.8820	−2.8393	2.0963	0.20
Δn_D	−0.0015	−0.0009	0.0002		0.0003
		DBE + Cyclohexane			
V^E(cm^3·mol^{-1})	1.6099	−0.5441	0.3097	- 0.0972	0.04
$\Delta\mu_D$ (mPa·s)	−0.3441	0.2002	−0.1375	0.0778	0.20
Δn_D	−0.0174	0.0061	−0.0019	0.0008	0.0003
		2-Butanol + Cyclohexane			
V^E(cm^3·mol^{-1})	2.5070	−0.9128	0.3205	0.5590	0.03
$\Delta\mu_D$ (mPa·s)	−3.4626	−1.6108	−0.9026	−0.1447	0.15
Δn_D	−0.0076	−0.0013	−0.0039	0.0068	0.0026

$$\mathrm{AAD} = \frac{100}{N}\sum_{i=1}^{N}\left|\frac{\rho_i^{\mathrm{exp}} - \rho_i^{\mathrm{calc}}}{\rho_i^{\mathrm{exp}}}\right| \quad (15)$$

with N as the number of measured data.

Table 3 shows the density (ρ), dynamic and kinematic viscosities (μ_D and μ_c), and refractive index (n_D) experimental data for the studied binary mixtures. It is noted that the refractive index of the binary mixture DBE (1) + 2-butanol (2) present the same experimental value of the refractive index for several molar fractions because the difference between the refractive index of DBE and that of 2-butanol is less than the measurement uncertainty of this quantity.

Table 4 also lists the sets of coefficients A_i and C_i used to fit the measured values of ρ and μ_D using polynomial equations eqs 5 and 6.

Table 5 lists the sets of adjustable coefficients D_i required to correlate V^E, $\Delta\mu D$, or Δn_D using the Redlich−Kister (eq 10).

The AADs between experimental densities and modeled by using the PC-SAFT EoS are provided in Table 6. The AADs for dibutyl ether (DBE), 2-butanol, and cyclohexane, respectively, are 0.004, 0.04, and 0.01%.

The variation of density as a function of mole fraction for binary mixtures of DBE (1) + 2-butanol (2), 2-butanol (1) + cyclohexane (2), and DBE (1) + cyclohexane (2) is shown in Figure 1. Table 3 shows that the density values for the binary mixtures DBE (1) + 2-butanol (2) and DBE (1) + cyclohexane (2) decrease as the mole fraction x_1 increases, whereas the density values for the binary mixture 2-butanol (1) + cyclohexane (2) increase as x_1. The experimental density

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J. Chem. Eng. Data XXXX, XXX, XXX−XXX

Table 6. Characteristic Parameters of PC-SAFT Equation of State for Dibutyl Ether (DBE), 2-Butanol, and Cyclohexane

compound	m [−]	σ [A]	ε/k [K]	ε^{HB}/k [K]	K^{HB} [K]	AAD % (ρ^{liq})
dibutyl ether	4.87667	3.57715	226.132			0.004
2-butanol	3.68544	3.21794	213.009	2085.52	0.0312056	0.04
cyclohexane	3.1869	3.5318	246.7918			0.01

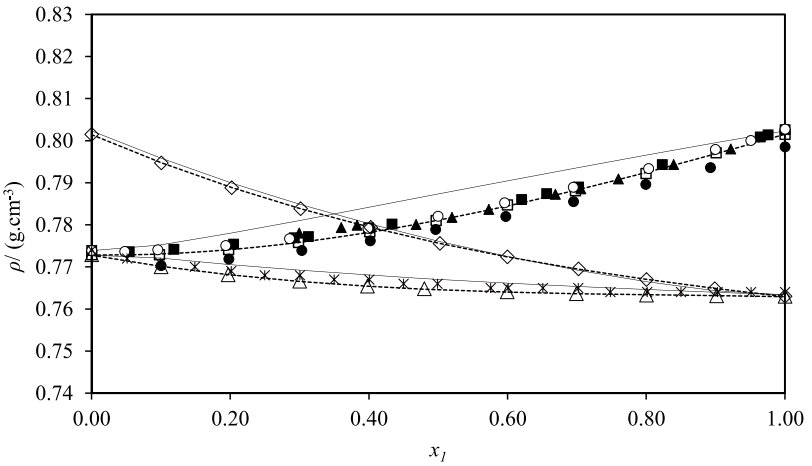

Figure 1. Experimental values of density, ρ, as a function of mole fraction of x_1 for binary mixtures: (open diamond), DBE (1) + 2-butanol (2); (open square), 2-butanol (1) + cyclohexane (2); (open triangle), DBE (1) + cyclohexane (2) at 298.15 K and at 0.1 MPa. For 2-butanol (1) + cyclohexane (2): (open circle), ref 58; (shaded circle), ref 59; (shaded square), ref 68; (shaded triangle), ref 67; (zhe), ref 15. The polynomial equation (eq 5) is presented with a dashed line, and the PC-SAFT equation is presented with a solid line.

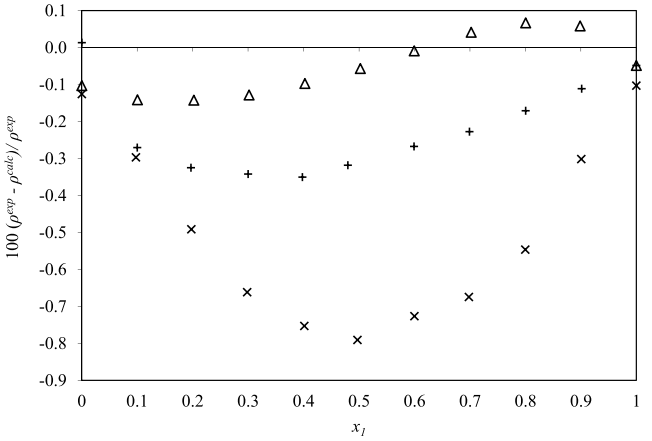

Figure 2. Deviations between measured and calculated densities with the PC-SAFT equation at 298.15 K. For (open triangle), DBE (1) + 2-butanol (2); (multiplication sign), 2-butanol (1) + cyclohexane (2); and (plus sign), DBE (1) + cyclohexane (2) vs mole fraction at 0.1 MPa.

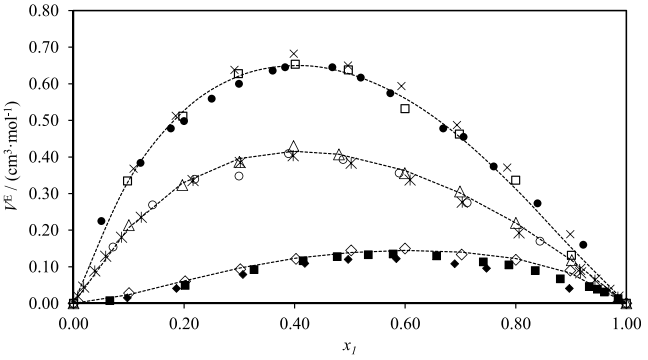

Figure 3. Excess molar volumes, V^E, as a function of mole fraction of x_1 for binary mixtures: (open diamond), DBE (1) + 1-butanol (2); (open square), 2-butanol (1) + cyclohexane (2); (open triangle), DBE (1) + cyclohexane (2) at 298.15 K and at 0.1 MPa. For (shaded circle), ref 67; (multiplication sign), ref 58; (shaded diamond), ref 71; (shaded square), ref 69; (zhe), ref 70; (open circle), ref 72. The Redlich−Kister correlation is presented with a dashed line.

values for binary mixture 2-butanol (1) + cyclohexane (2) were compared to values given by Abala et al.,[15] Morrone and Francesconi,[67] González al.,[58] Gama and Tojo,[68] and Oswal et al.[59] As seen in Figure 1, there is a high level of agreement. Moreover, experimental data of refractive index for the binary mixtures DBE (1) + cyclohexane (2) and 2-butanol (1) + cyclohexane (2) are compared to data previously published by Abala et al.,[15] Gilani et al.,[76] and Gama and Tojo[68] for the same binary mixtures. The comparison presents a high level of agreement for the first binary mixture (DBE (1) + cyclohexane (2)) with Abala et al.,[15] with an AAD of 0.05%; also, the comparison shows a good agreement for the second binary mixture (2-butanol (1) + cyclohexane (2)) with Gilani et al.[76] and Gama and Tojo,[68] with an AAD of 0.04 and 0.42%, respectively.

Figure 1 shows also densities predicted using the PC-SAFT equation of state. The AAD for binary mixtures of DBE (1) + 2-butanol (2), 2-butanol (1) + cyclohexane (2), and DBE (1) + cyclohexane (2) is within [0.009−0.14%], [0.12−0.97%], and [0.04−0.35%] as shown in Figure 2. The densities correlated by the PC-SAFT equation of state exhibit poor agreement for mixing over measured data because the binary interaction parameters are assumed to be zero for the mixtures.

Figure 3 represents the changes in excess molar volumes as a function of the mole fraction x_i for the three binary mixtures. It demonstrates that V^E values are positive over a wide range of composition. Binary mixtures such as DBE (1) + 2-butanol (2) and 2-butanol (1) + cyclohexane (2) have one strong self-

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J. Chem. Eng. Data XXXX, XXX, XXX−XXX

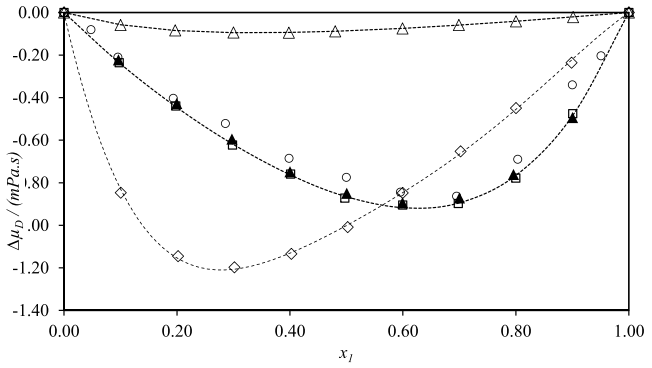

Figure 4. Deviations in dynamic viscosity, $\Delta\mu_D$, as a function of mole fraction of x_1 for binary mixtures: (open diamond), DBE (1) + 1-butanol (2); (open square), 2-butanol (1) + cyclohexane (2); (open triangle), DBE (1) + cyclohexane (2) at 298.15 K and at 0.1 MPa. For (shaded triangle), ref 73 for 2-butanol (1) + cyclohexane (2); (open circle), ref 58 for 2-butanol (1) + cyclohexane. The Redlich−Kister correlation is presented with a dashed line.

associating component (alcohol) and two non-self-associating components (DBE and cyclohexane) that can form hydrogen bonding associations with the alcohol. The breakdown of hydrogen bonds in alcohol causes a volume expansion in the mixtures, which yields the positive term. The abovementioned sequence is reversed as maximum values shift toward larger concentrations of DBE and cyclohexane.

The excess volume values V^E for the DBE (1) + cyclohexane (2) binary mixture are positive. Due to the absence of association effects, it is hypothesized that the cohesiveness between DBE and cyclohexane is insignificant (hydrogen bonds, double bonds, etc.). The positive contribution to V^E for these mixtures could be due to disturbance in the hydrocarbon orientation order or breakdown of cohesive forces, as well as the steric effect, which prevents pure components from being in close proximity. Excess molar volume tendency curves for binary mixtures of DBE (1) + 2-butanol (2) and 2-butanol (1) + cyclohexane (2) were compared to those produced by Morrone and Francesconi,[67] González et al.,[58] Bernazzani et al.,[69] and Kammerer and Lichtenthaler.[71] At all compositions, this comparison reveals a high level of agreement. Furthermore, the comparison of experimental excess molar volume values with those reported by Berti et al.[70] and Teng and Acree[72] for DBE (1) + cyclohexane (2) indicates good agreement between both sets of data at all compositions.

Figure 4 shows plots of $\Delta\mu_D$ derived from experimental data for three binary mixtures; additionally, the literature values[73,63] and our results are in good agreement. Over the entire range of composition, the variations in dynamic viscosity of these mixtures are negative. For the binary mixture of DBE (1) + cyclohexane (2), the lowest $\Delta\mu_D$ value comes at mole fraction $x_1 = 0.47$. The internal friction force of this combination lowers as a result of the lower interaction between dissimilar molecules, resulting in negative viscosity deviations.

The $\Delta\mu_D$ vs x_1 curves for alkanol-containing systems indicate the minimal value at mole fraction $x_1 = 0.3$ for the binary mixture DBE (1) + 2-butanol (2) and the minimum value at mole fraction $x_1 = 0.6$ for the binary mixture 2-butanol (1) + cyclohexane (2). The alteration of hydrogen bonding is the key factor affecting the fluctuations in $\Delta\mu_D$ values of these binary mixtures.

Table 7. Density, ρ, Dynamic viscosity, μ_D, Kinematic Viscosity, μ_c, and Refractive Index, n_D, for the Ternary Mixtures $\{x_1$ DBE + x_2 2-Butanol + $(1 - x_1 - x_2)$ Cyclohexane$\}$ at T = 298.15 K and at p = 0.1 MPa[a]

x_1	x_2	ρ (g·cm^{-3})	μ_D (mPa·s)	μ_c(mm^2·s^{-1})	n_D
0.0000	0.0000	0.7729	0.91	1.18	1.42337
0.1008	0.0996	0.7705	0.82	1.07	1.41515
0.1007	0.2009	0.7721	0.85	1.10	1.41217
0.0996	0.2961	0.7741	0.89	1.15	1.40948
0.1011	0.3981	0.7764	0.95	1.23	1.40686
0.1005	0.5013	0.7795	1.06	1.36	1.40422
0.1036	0.5968	0.7826	1.19	1.36	1.40194
0.1014	0.6985	0.7865	1.40	1.78	1.39958
0.0990	0.7766	0.7895	1.60	2.03	1.39799
0.2004	0.1014	0.7689	0.78	1.01	1.41148
0.2010	0.1993	0.7706	0.81	1.05	1.40884
0.2019	0.2990	0.7727	0.84	1.09	1.40603
0.2021	0.3978	0.7751	0.90	1.16	1.40382
0.2015	0.4973	0.7781	0.99	1.27	1.40165
0.2012	0.5967	0.7813	1.11	1.42	1.39949
0.2015	0.6976	0.7851	1.27	1.62	1.39714
0.3017	0.1012	0.7677	0.75	0.97	1.40788
0.2997	0.2016	0.7696	0.77	1.00	1.40587
0.3019	0.3116	0.7720	0.82	1.06	1.40335
0.3015	0.3976	0.7742	0.87	1.12	1.40145
0.3014	0.4965	0.7771	0.94	1.21	1.39927
0.3027	0.5981	0.7803	1.05	1.34	1.39724
0.3984	0.0969	0.7668	0.72	0.94	1.40567
0.4013	0.1921	0.7685	0.75	0.97	1.40357
0.4017	0.3004	0.7710	0.79	1.02	1.40113
0.4027	0.3981	0.7734	0.84	1.08	1.39917
0.4032	0.4996	0.7764	0.91	1.17	1.39711
0.5030	0.0969	0.7661	0.71	0.92	1.40334
0.4989	0.1996	0.7681	0.73	0.95	1.40130
0.5057	0.2975	0.7703	0.77	1.00	1.39903
0.4999	0.4023	0.7730	0.82	1.06	1.39726
0.6000	0.0971	0.7656	0.70	0.91	1.40128
0.6028	0.1956	0.7675	0.72	0.94	1.39929
0.6009	0.2902	0.7698	0.75	0.98	1.39739
0.7029	0.0991	0.7652	0.69	0.90	1.39935
0.7074	0.1827	0.7669	0.70	0.92	1.39769
0.8171	0.1005	0.7650	0.68	0.89	1.39745
1.0000	0.0000	0.7630	0.66	0.86	1.39655
0.0000	1.0000	0.8015	3.13	3.91	1.39517

[a]Standard uncertainties u are $u(T)$ = 0.04 K and $u(p)$ = 0.01 MPa, and the combined expanded uncertainties U in density, dynamic viscosity, kinematic viscosity, and refractive index are $U(\rho)$ = 0.0005 g·cm^{-3}, $U(\mu_D) = 0.02\ \mu_D$, $U(\mu_c) = 0.03\ \mu_c$, and $U(n_D)$ = 0.00005, respectively (0.95 level of confidence).

The presence of non-polar molecules breaks the hydrogen bonds between 2-butanol molecules, causing the self-association of 2-butanol molecules to dissociate. As a result, the mixture's fluidity is superior to that of 2-butanol in its pure state on a macroscopic level.

5.2. Thermophysical Properties of Ternary Mixtures. Table 7 shows the experimental densities, dynamic and kinematic viscosities, and refractive indices of DBE (1) + 2-butanol (2) + cyclohexane (3) as a function of mole fraction x_i. Table 8 contains also the sets of coefficients used to fit the measured data of ρ using a polynomial equation (eq 12).

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J. Chem. Eng. Data XXXX, XXX, XXX−XXX

Table 8. Coefficients B_{ij} Needed for the Polynomial Eq 12 with Standard Deviations Obtained for the Studied Ternary Mixtures in This Work at T = 298.15 K and at p = 0.1 MPa

	$B_{(11)}$	$B_{(21)}$	$B_{(31)}$	$B_{(41)}$	$B_{(12)}$	$B_{(22)}$	$B_{(32)}$	$B_{(42)}$	$B_{(13)}$	$B_{(23)}$	$B_{(33)}$	$B_{(43)}$	σ
ρ (g·cm^{-3})	0.7521	0.0215	−0.0137	0.0029	0.7783	0.0453	−0.0502	0.0288	0.7692	0.0052	−0.0106	0.0090	0.00003

Table 9. The Fitting Parameters F_i Corresponding to the Cibulka Equation (14) for the Studied Ternary Mixture

Δ_{123}	F_0	F_1	F_2	σ
V^E(cm^3·mol^{-1})	−0.5692	−2.6747	4.8100	0.0032
$\Delta\mu_D$ (mPa·s)	1.05	0.75	9.51	0.0033
Δn_D	0.100	0.018	−1.446	0.0007

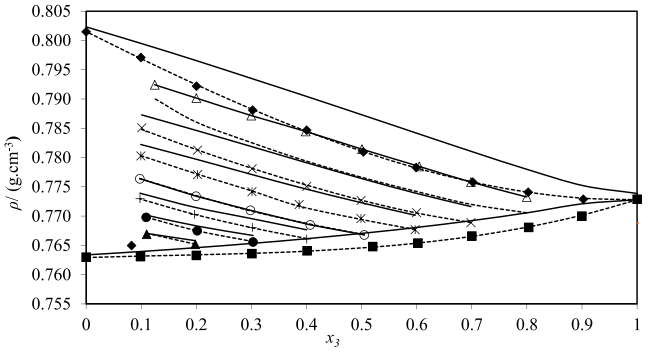

Figure 5. Experimental values of density, ρ, as a function of mole fraction of x_3 for the ternary mixture: DBE (1) + 2-butanol (2) + cyclohexane (3); (open triangle), x_1 = 0.1; (multiplication sign), x_1 = 0.2; (zhe), x_1 = 0.3; (open circle), x_1 = 0.4; (plus sign), x_1 = 0.5; (shaded circle), x_1 = 0.6; (shaded triangle), x_1 = 0.7; (shaded diamond), x_1 = 0.8; (shaded square), $x_3 = x_2$ for the binary mixture DBE (1) + cyclohexane (2); (shaded diamond), $x_3 = x_2$ for the binary mixture 2-butanol (1) + cyclohexane (2). The polynomial equation (eq 12) is presented with a dashed line, and the PC-SAFT equation of state is presented with a solid line.

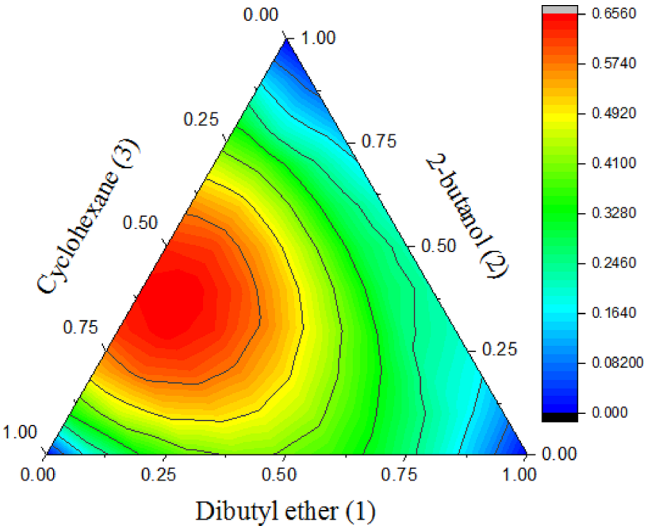

Figure 6. Contour lines of excess molar volumes, V^E (cm^3·mol^{-1}), for the ternary mixture DBE (1) + 2-butanol (2) + cyclohexane (3) using eqs 13 and 14 at 0.1 MPa and at 298.15 K.

Table 9 shows the sets of adjustable coefficients required to correlate V^E, $\Delta\mu_D$, or Δn_D using eqs 13 and 14. Figure 5 shows the experimental density values as a function of mole fraction of x_3 for the ternary mixture DBE (1) + 2-butanol (2) + cyclohexane (3). This graphic includes also densities predicted using the PC-SAFT equation of state, which demonstrates a good agreement with experimental data for the examined ternary mixture.

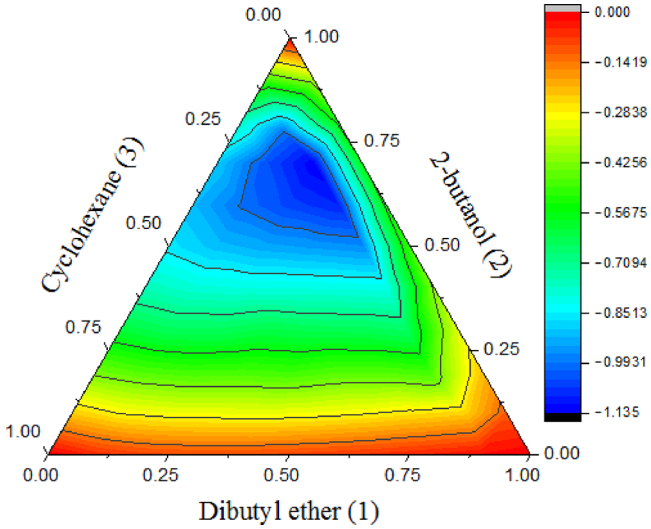

Figure 7. Contour lines of deviations in dynamic viscosity, $\Delta\mu_D$ (mPa·s), for the ternary mixture DBE (1) + 2-butanol (2) + cyclohexane (3) using eqs 13 and 14 at 0.1 MPa and at 298.15 K.

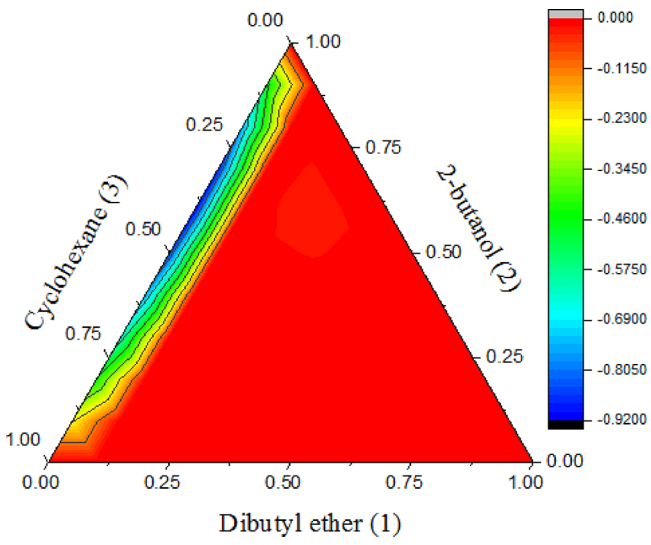

Figure 8. Contour lines of deviations in the refractive index, Δn_D, for the ternary mixture DBE (1) + 2-butanol (2) + cyclohexane (3) using eqs 13 and 14 at 0.1 MPa and at 298.15 K.

Overall, the V^E values for the examined ternary mixture are positive at T = 298.15 K, as presented in Figure 6. Positive V^E values can be explained by the breaking effect mechanism between the mixtures of 2-butanol (1) + cyclohexane (2) or DBE (1) + 2-butanol (2). However, due to the breaking of hydrogen bonds in alcohol, a volume expansion in the mixture occurs, which generates the positive term. The V^E of the mixture DBE (1) + cyclohexane (2) are positive over the

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J. Chem. Eng. Data XXXX, XXX, XXX−XXX

whole range of mole fraction, and it is proposed that the cohesion between cyclohexane and DBE is negligible because of the absence of the association effects. The positive values of V^E for these studied mixtures are justified by the breaking of cohesion forces or the disruption in the orientation order of the hydrocarbon, and can be justified also by the steric effect, that prevent the proximity of pure components.

Figure 7 shows the dynamic viscosity deviations against the molar fraction for the ternary mixture at 298.15 K. The values of $\Delta\mu_D$ are clearly negative over the entire range composition, which can be explained by the destruction of hydrogen bonds and dispersion force. Observations at 298.15 K were expected to exhibit negative values of deviations in the refractive index, (Δn_D) due to the ternary mixture interactions, as shown in Figure 8. A negative value of Δn_D demonstrates that the refractive index deviations of the liquid mixture are impacted not only by the strength of the specific interaction but also by the molecular size and shape of the components that composed the mixture. In the experimental measurement of the mixtures, the behavior of V^E has an opposite tendency compared to the Δn_D, considering that the decline of V^E values derives from the increase in the number of dipoles per unit volume.[75]

6. CONCLUSIONS

Density, (ρ), dynamic and kinematic viscosities, (μ_D and μ_c), and refractive index, (n_D), measurements of the ternary mixtures dibutyl ether (1) + 2-butanol (2) + cyclohexane (3) and their corresponding binary mixtures over the whole range of composition was carried out. Based on the collected data, the excess molar volumes, (V^E), dynamic viscosity deviations, ($\Delta\mu_D$), and refractive index deviations, (Δn_D) of these mixtures were also computed. The Redlich−Kister equation was used to fit the V^E, $\Delta\mu_D$, and Δn_D for binary mixture compositions, while the Cibulka semi-empirical equation was used to fit the ternary mixtures. The structural effects and intermolecular forces presented in the studied mixtures can be analyzed using the values of V^E, $\Delta\mu_D$, and Δn_D. In order to determine the values of V^E in alkanol-containing systems, the process of breaking hydrogen bonds between 2-butanol molecules and geometrical interstitial accommodation are fundamental aspects. The PC-SAFT EoS agrees well with the measured density data for the studied binary and ternary mixtures. These results are crucial for further research into gasoline additives.

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Notes

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LIST OF SYMBOLS

ρ (g/cm^3)	density
μ_D (mPa·s)	dynamic viscosity
μ_c (mm^2·s^{-1})	kinematic viscosity
n_D	refractive index
V^E (cm^3·mol^{-1})	excess molar volume
$\Delta\mu_D$(mPa·s)	dynamic viscosity deviation
Δn_D	refractive index deviation
T (K)	temperature
p (MPa)	pressure
x_i	mole fraction
i	constituent identification
EoS	equation of state

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