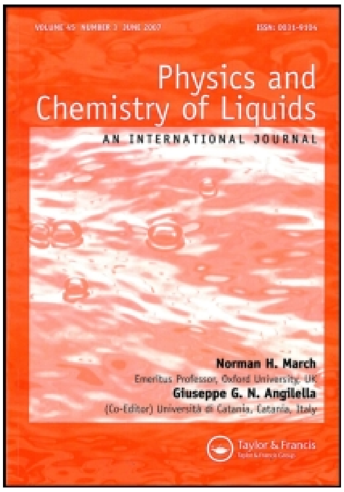

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Experimental and theoretical studies of viscosities of ternary mixture [2-propanol ethyl acetate *n*-hexane] and its binary constituents at 298.15, 308.15 and 313.15 K

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Experimental and theoretical studies of viscosities of ternary mixture [2-propanol + ethyl acetate + *n*-hexane] and its binary constituents at 298.15, 308.15 and 313.15 K

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The viscosities of the ternary mixture [2-propanol + ethyl acetate + *n*-hexane] and its binary constituents; [2-propanol + ethyl acetate], [2-propanol + *n*-hexane] and [ethyl acetate + *n*-hexane] were measured over the whole concentration range at three temperatures 298.15, 308.15 and 313.15 K. The M_4 cubic equation of state due to Mohsen-Nia *et al.* (M. Mohsen-Nia, H. Modarress, G.A. Mansoori. *Fluid Phase Equilibria*, **206**, 27 (2003)) was used along with the modified Eyring kinematic viscosity model to correlate the measured viscosity data and the interaction parameters for the binary mixtures are reported. The binary interaction parameters were successfully used for viscosity calculation of the ternary mixture.

Keywords: Viscosity; 2-Propanol; Ethyl acetate; *n*-Hexane; Equation of state; Eyring viscosity model

1. Introduction

The organic solvent mixtures are important chemicals for the different industrial purposes such as solvent extraction of aromatic hydrocarbons from alkanes [1,2], crystallization and extraction of pure organic and mineral salts from aqueous mixtures [3,4] and solvent cleaning processes [5], therefore, measurements and modeling of thermodynamic and transport properties of the binary and ternary solvent mixtures have considerable current interest in chemical engineering research fields.

In design and operation of chemical processes, viscosities of pure and liquid mixtures are essential quantities. Viscosity data can be used to clarify the structural arrangement of pure and liquid mixtures at the molecular level [6]. Unfortunately, the viscosity data and suitable model for prediction of viscosity of binary and especially ternary and higher multi-components mixtures are scarce.

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The ternary mixture of solvents; [2-propanol (1) + ethyl acetate (2) + n-hexane (3)] containing two highly polar components (1, 2) in the non-polar solvent (3) can be considered as a suitable mixed solvent for the different industrial processes.

In this work, the viscosities of the ternary solvent mixture [2-propanol (1) + ethyl acetate (2) + n-hexane (3)] and its binary constituent mixtures were measured at three temperatures 298.15, 308.15 and 313.15 K and over the whole concentration range.

In the lack of data for viscosity of liquid mixtures the only way left is to choose one of the available semi-empirical models, which are based either on corresponding state principle [7] or on the Eyring theory [8], for predicting the viscosity of liquid mixtures.

The cubic equations of state have an important role in predicting the thermodynamic quantities. But when it comes to transport properties such as viscosity, there are only a few models based on equation of state approach for their prediction. Lee *et al.* [9] have presented a new viscosity model that estimates the excess activation free energy of flow, $G^{\#\mathrm{E}}$ in Eyring theory with the aid of Patel and Teja equation of state [10]. Giro *et al.* [11] have used a modified Redich–Kwong–Soave equation on state due to Fuller [12] with the Eyring viscosity model to correlate viscosities of binary mixtures. Also by using the binary interaction parameters they have calculated the viscosity of ternary liquid mixtures.

In this work, we have correlated the measured binary and ternary mixtures viscosities by using M_4 equation on state [13] with the Eyring viscosity model. The calculated binary interaction parameters k_{ij} of the binary mixtures of [2-propanol (1) + ethyl acetate (2)], [(2-propanol (1) + n-hexane (3)] and [ethyl acetate (2) + n-hexane (3)] have been used for the correlation of the viscosity of the studied ternary mixtures. The results of these calculations indicate the capability of the used model in viscosity predictions of fluid mixtures.

The detailed theory in derivation of the necessary equations used in viscosity calculations with the aid of M_4 equation of state is described in following section.

2. Theory

According to the Eyring viscosity model, [8, 9] the viscosity can be calculated by the expression:

$$(\eta V)_{\mathrm{mix}} = (\eta V)_{\mathrm{id}} \exp\left(\frac{G^{\#\mathrm{E}}}{RT}\right), \tag{1}$$

where R is the gas constant, T the absolute temperature and

$$(\eta V)_{\mathrm{id}} = \exp\left[\sum_i x_i \ln\left(\eta_i^* V_i^*\right)\right]. \tag{2}$$

where x_i is the mole fraction of component i.

In equations (1) and (2), $(\eta V)_{\mathrm{mix}}$ and $(\eta V)_{\mathrm{id}}$ are respectively the kinematic viscosities of real and ideal mixtures at the pressure P and temperature T and $(\eta_i^* V_i^*)$ is the kinematic viscosity of pure component i. $G^{\#\mathrm{E}}$ in equation (1) is the excess Gibbs energy of viscous flow required to move one mole of the fluid particles from a stable state to an activated state. From equations (1) and (2) the following equation can be obtained:

$$G^{\#\mathrm{E}} = RT\left[\ln(\eta V)_{\mathrm{mix}} - \sum_i x_i \ln\left(\eta_i^* V_i^*\right)\right], \tag{3}$$

where V and V_i^* are respectively the mixture and pure component i molar volumes. There is a certain similarity between the excess Gibbs energy of viscous flow $G^{\#\mathrm{E}}$ and the thermodynamic G^{E} which makes $G^{\#\mathrm{E}} = G^{\mathrm{E}}$ a reasonable assumption [11]. Therefore, $G^{\#\mathrm{E}}$ can be calculated alternatively by the thermodynamic expression for G^{E} using an equation of state. The thermodynamic G^{E} is given as [14, 15]:

$$G^{\mathrm{E}} = RT\sum_i x_i\left(\ln\phi_i - \ln\phi_i^*\right). \tag{4}$$

where ϕ_i and ϕ_i^* are the fugacity coefficients of component i in the mixture and in the pure state respectively.

Therefore, from equations (2)–(4) the following equation is obtained:

$$(\nu)_{\mathrm{mix}} = (\nu)_{\mathrm{id}} \exp\sum_i x_i\left(\ln\phi_i - \ln\phi_i^*\right) \tag{5}$$

where, for the sake of abbreviation the kinematic viscosities $(\eta V)_{\mathrm{mix}}$ and $(\eta V)_{\mathrm{id}}$ are respectively presented by ν_{mix} and ν_{id}.

The M_4 equation of state is of the following form [13]:

$$P = \frac{RT}{V}\left(\frac{V+\alpha b}{V-b}\right) - \frac{a}{T^{1/2}V(V+2\alpha b)} \quad \text{and} \quad \alpha = 1.3191 \tag{6}$$

where the parameters a and b for the mixture are expressed as simple one-parameter van der Waals one-fluid (vdW-1) mixing rule [14]:

$$a = \sum_i\sum_j x_i x_j (1-k_{ij})(a_i a_j)^{1/2} \tag{7}$$

$$b = \sum_i x_i b_i \tag{8}$$

k_{ij} in equation (7) is the binary interaction parameter. The expressions for the fugacity coefficients (ϕ_i and ϕ_i^*) corresponding to the M_4 equation are given in Appendix A.

3. Experimental

n-Hexane, 2-propanol and ethyl acetate (purities > 99%), were supplied by Aldrich. Therefore, all chemicals were used without further purification.

Kinematic viscosities, ν of the pure compounds and their mixtures were measured using an Ubbelohde viscosimeter (inner diameter = 0.36 mm). The flow time was measured with a stop watch capable of recording to 0.01 s. For each mixture, at least four flow time measurements were performed and the results were averaged.

The viscosimeter was calibrated with by means of the equation:

$$\nu = \frac{\eta}{\rho} = Kt - \frac{L}{t} \tag{9}$$

where ν is the kinematic viscosity, η is the absolute viscosity, ρ is the density and t is the flow time of the calibration solution. The values of the characteristic viscometer constants K and L were determined as: $0.5845 \times 10^{-2}\,\mathrm{m^2 s^{-2}}$ and $0.4905\,\mathrm{m^2}$, respectively. The mixtures were prepared by mass using an analytical balance with a precision of $\pm 0.1\,\mathrm{mg\,g cm^{-3}}$. The precision in viscosity measurements was ± 0.01 mPa s.

In viscosity measurements, the temperature of the samples was controlled by using a water bath equipped with a thermostat of accuracy of ±0.1 K.

4. Results and discussion

Viscosity of the studied pure compounds at different temperatures and atmospheric pressure were measured. The measured viscosities are shown in table 1. In this table, the obtained data are compared with the available viscosity data in literature [16–19]. These comparisons indicated good consistency between these results and those presented in the literature. The measured kinematic viscosities ν, for the studied binary and ternary mixtures are given in tables 2–4.

For the correlation of the measured viscosities by the M_4 equation of state and Eyring viscosity model (equation (5)), the fugacity coefficient ϕ_i was calculated by M_4 equation of state as presented in Appendix A. The simple one-parameter

Table 1. Measured viscosities of the pure components at different temperatures and atmospheric pressure.

Components	T (K)	η (mPa s)
2-Propanol	298.15	2.0400
	298.15	2.0435[a]
	298.15	2.0436[b]
	308.15	1.5673
	313.15	1.3664
Ethyl acetate	298.15	0.4318
	298.15	0.4230[c]
	308.15	0.3864
	313.15	0.3691
n-Hexane	298.15	0.2973
	298.15	0.3000[c]
	298.15	0.2940[b]
	308.15	0.2715
	313.15	0.2589

[a] Experimental data [16].
[b] Experimental data [17].
[c] Experimental data [18].

Table 2. Experimental $(\nu)_{\mathrm{exp.}}$ and calculated $(\nu)_{\mathrm{calc.}}$ for 2-propanol (1) + ethyl acetate (2) + *n*-hexane (3) mixtures at 298.15 K and atmospheric pressure ($k_{12} = -0.115$, $k_{13} = -0.125$, $k_{23} = -0.0191$).

x_1	x_2	$(\nu)_{\mathrm{exp.}}$	$(\nu)_{\mathrm{calc.}}$	RE%	x_1	x_2	$(\nu)_{\mathrm{exp.}}$	$(\nu)_{\mathrm{calc.}}$	RE%
0.0224	0.9450	0.4474	4773	6.6	0.7582	0.2418	1.113	1.1743	5.5
0.0415	0.3631	0.4386	0.4428	1.0	0.8686	0.1314	1.5248	1.6238	6.5
0.0537	0.0369	0.4548	0.4628	1.8	0.9636	0.0364	2.2215	2.2661	2.0
0.1081	0.0759	0.4638	0.4752	2.4	0.0372	0.0000	0.4582	0.4626	1.0
0.1788	0.7171	0.5004	0.4933	−1.4	0.1351	0.0000	0.4754	0.4909	3.3
0.1947	0.0927	0.4719	0.5029	6.7	0.2152	0.0000	0.5006	0.5204	4.0
0.2232	0.7504	0.5250	0.5149	−1.9	0.3546	0.0000	0.5682	0.5918	4.2
0.2432	0.1556	0.5006	0.5172	3.3	0.4060	0.0000	0.6028	0.6271	4.0
0.3033	0.6018	0.5462	0.5403	−1.1	0.5723	0.0000	0.8147	0.7946	−2.5
0.3304	0.3882	0.5404	0.5495	1.7	0.6165	0.0000	0.8813	0.8593	−2.5
0.3516	0.3579	0.5485	0.5626	2.5	0.7122	0.0000	1.0859	1.0467	−3.6
0.4145	0.5391	0.6130	0.6111	−0.3	0.8948	0.0000	1.8120	1.7455	−3.7
0.4844	0.4187	0.6096	0.6689	9.7	0.9289	0.0000	2.0214	1.9695	−2.6
0.4965	0.3094	0.6629	0.6806	2.7	0.0000	0.0987	0.4427	0.4456	0.7
0.5182	0.3614	0.6881	0.7043	2.3	0.0000	0.1581	0.4396	0.4418	0.5
0.5520	0.2475	0.7374	0.7463	1.2	0.0000	0.2246	0.4346	0.4483	0.9
0.6368	0.0583	0.8817	0.8860	0.5	0.0000	0.3465	0.4347	0.4343	−0.09
0.6787	0.2543	0.9240	0.9612	4.0	0.0000	0.4906	0.4330	0.4337	0.2
0.7114	0.0992	1.0415	1.0370	−0.4	0.0000	0.5977	0.4405	0.4367	−0.9
0.7613	0.1419	1.1236	1.1751	4.6	0.0000	0.6444	0.4392	0.4391	−0.02
0.8006	0.1785	1.2394	1.3100	5.7	0.0000	0.7507	0.4454	0.4468	0.3
0.8266	0.1235	1.3562	1.4157	4.3	0.0000	0.8015	0.4511	0.4520	0.2
0.9006	0.0355	2.0393	1.7877	−12.3	0.0000	0.9502	0.4732	0.4730	−0.04
0.0470	0.9530	0.4970	0.4850	−2.4					
0.1635	0.8365	0.5125	0.5022	−2.0					
0.2252	0.7748	0.5336	0.5188	−2.8					
0.3192	0.6808	0.5715	0.5566	−2.6					
0.4162	0.5838	0.6257	0.6161	−1.5					
0.5682	0.4318	0.7575	0.7728	2.0					
0.6716	0.3284	0.9104	0.9508	4.4					

van der Waals one-fluid (vdW-1) mixing rules as represented by equations (7) and (8) were used. The kinematic viscosities for the mixtures $\nu_{\mathrm{mix}} = (\eta V)_{\mathrm{mix}}$ were calculated by using equation (5). The kinematic viscosities of ideal mixtures $\nu_{\mathrm{id}} = (\eta V)_{\mathrm{id}}$ were calculated by using the kinematic viscosities of pure components $\nu_i^* = (\eta_i^* V_i^*)$ in equation (2). The interaction parameters k_{ij} in equation (7) for the studied binary mixtures were obtained by minimizing the average absolute deviation, AAD(%), as presented by the following equation:

$$\mathrm{AAD}\% = \frac{1}{N}\sum_{k=1}^{N} \frac{\left|\nu_{\mathrm{calc.}} - \nu_{\mathrm{exp.}}\right|_k}{\nu_{\mathrm{exp.},k}} \times 100, \tag{10}$$

where the superscripts "calc." and "exp." refer to the calculated and experimental values of the kinematic viscosities.

The calculated viscosities are compared with measured results in tables 2–4. According to these tables the average absolute deviations percent (AAD%) for the studied binary mixtures is about 2%. By using the calculated interaction parameters, k_{ij}, of the binary mixtures, in equation (7), the parameter a of M_4 equation of state for the ternary mixture of [2-propanol (1) + ethyl acetate (2) + *n*-hexane (3)] at different compositions was calculated and then from equation (5) by the same procedure as

Table 3. Experimental $(\nu)_{\mathrm{exp.}}$ and calculated $(\nu)_{\mathrm{calc.}}$ for 2-propanol (1) + ethyl acetate (2) + *n*-hexane (3) mixtures at 308.15 K and atmospheric pressure ($k_{12} = -0.114$, $k_{13} = -0.1245$, $k_{23} = -0.019$).

x_1	x_2	$(\nu)_{\mathrm{exp.}}$	$(\nu)_{\mathrm{calc.}}$	RE%	x_1	x_2	$(\nu)_{\mathrm{exp.}}$	$(\nu)_{\mathrm{calc.}}$	RE%
0.0224	0.9450	0.4343	0.4320	−0.5	0.7582	0.2418	0.9357	0.9692	3.6
0.0415	0.3631	0.4025	0.4052	0.6	0.8686	0.1314	1.2303	1.3062	6.2
0.0537	0.0369	0.4182	0.4246	1.5	0.9636	0.0364	1.7163	1.7766	3.5
0.1081	0.0759	0.4255	0.4325	1.6	0.0372	0.0000	0.4209	0.4247	0.9
0.1788	0.7171	0.4515	0.4424	−2.0	0.1351	0.0000	0.4359	0.4454	2.2
0.1947	0.0927	0.4435	0.4529	2.1	0.2152	0.0000	0.4546	0.4675	2.8
0.2232	0.7504	0.4736	0.4593	−3.0	0.3546	0.0000	0.5055	0.5219	3.2
0.2432	0.1556	0.4546	0.4629	1.8	0.4060	0.0000	0.5350	0.5489	2.6
0.3033	0.6018	0.4923	0.4800	−2.5	0.5723	0.0000	0.6797	0.6778	−0.03
0.3304	0.3882	0.4848	0.4862	0.3	0.6165	0.0000	0.7371	0.7274	1.3
0.3516	0.3579	0.4933	0.4964	0.6	0.7122	0.0000	0.8949	0.8705	−2.7
0.4145	0.5391	0.5438	0.5763	6.0	0.8948	0.0000	1.4226	1.3935	−2.0
0.4844	0.4187	0.5416	0.5795	7.0	0.9289	0.0000	1.5749	1.5586	−1.0
0.4965	0.3094	0.5835	0.5885	0.9	0.0000	0.0987	0.4088	0.4107	0.5
0.5182	0.3614	0.6016	0.6071	0.9	0.0000	0.1581	0.4073	0.4069	−0.1
0.5520	0.2475	0.6423	0.6397	−0.4	0.0000	0.2246	0.4008	0.4034	0.6
0.6368	0.0583	0.7456	0.7477	0.3	0.0000	0.3465	0.3992	0.3992	0.0
0.6787	0.2543	0.7882	0.8059	2.2	0.0000	0.4906	0.3982	0.3978	−0.1
0.7114	0.0992	0.8648	0.8632	−0.2	0.0000	0.5977	0.4081	0.4091	0.2
0.7613	0.1419	0.9351	0.9687	3.6	0.0000	0.6444	0.4041	0.4015	−0.6
0.8006	0.1785	1.0230	1.0763	5.2	0.0000	0.7507	0.4111	0.4075	−0.9
0.8266	0.1235	1.1030	1.1501	4.2	0.0000	0.8015	0.4138	0.4117	−0.5
0.9006	0.0355	1.1411	1.4254	1.0	0.0000	0.9502	0.4310	0.4289	−0.5
0.0470	0.9530	0.4417	0.4378	−0.9					
0.1635	0.8365	0.4647	0.4721	1.6					
0.2252	0.7748	0.4875	0.4626	−5.1					
0.3192	0.6808	0.5105	0.4918	−3.7					
0.4162	0.5838	0.5560	0.5384	−3.2					
0.5682	0.4318	0.6607	0.6608	0.02					
0.6716	0.3284	0.7729	0.7985	3.3					

described for binary mixtures the kinematic viscosities of the ternary mixture were calculated. The results are shown in tables 2–4. Also in these tables the relative error RE% at each data point defined as

$$\mathrm{RE\%} = \frac{\nu_{\mathrm{calc.}} - \nu_{\mathrm{exp.}}}{\nu_{\mathrm{exp.}}} \times 100 \tag{11}$$

is reported.

Table 5 presents the k_{ij} and the AAD% for the studied binary mixtures. Table 6 presents the AAD% for the studied ternary mixture.

5. Conclusion

The viscosities of the ternary mixture [2-propanol (1) + ethyl acetate (2) + *n*-hexane (3)] and its binary mixtures constituents have been measured at three temperatures; 298.15, 308.15 and 313.15 K and atmospheric pressure.

The M_4 equation of state was incorporated with the modified Eyring viscosity model to predict viscosities for the studied mixtures. The mixture parameters of M_4 equation

Table 4. Experimental $(\nu)_{exp.}$ and calculated $(\nu)_{calc.}$ for 2-propanol (1) + ethyl acetate (2) + *n*-hexane (3) mixtures at 313.15 K and atmospheric pressure ($k_{12} = -0.11$, $k_{13} = -0.124$, $k_{23} = -0.0185$).

x_1	x_2	$(\nu)_{exp.}$	$(\nu)_{calc.}$	RE%
0.0224	0.9450	0.4151	0.4140	−0.2
0.0415	0.3631	0.3876	0.3906	0.7
0.0537	0.0369	0.4023	0.4087	1.6
0.1081	0.0759	0.4071	0.4149	1.9
0.1788	0.7171	0.4309	0.4239	−1.6
0.1947	0.0927	0.4230	0.4321	2.2
0.2232	0.7504	0.4502	0.4396	−2.3
0.2432	0.1556	0.4354	0.4406	1.2
0.3033	0.6018	0.4666	0.4568	−2.1
0.3304	0.3882	0.4596	0.4619	0.5
0.3516	0.3579	0.4698	0.4709	0.2
0.4145	0.5391	0.5195	0.5071	−2.4
0.4844	0.4187	0.5177	0.5465	5.6
0.4965	0.3094	0.5478	0.5529	0.9
0.5182	0.3614	0.5662	0.5704	0.7
0.5520	0.2475	0.6015	0.5973	−0.7
0.6368	0.0583	0.6899	0.6883	−0.2
0.6787	0.2543	0.7307	0.7455	2.0
0.7114	0.0992	0.7956	0.7901	−0.7
0.7613	0.1419	0.8596	0.8840	2.8
0.8006	0.1785	0.9356	0.9800	4.7
0.8266	0.1235	1.0058	1.0411	3.5
0.9006	0.0355	1.2523	1.2715	1.5
0.0470	0.9530	0.4234	0.4194	−0.9
0.1635	0.8365	0.4416	0.4310	−2.4
0.2252	0.7748	0.4589	0.4531	−1.3
0.3192	0.6808	0.4821	0.4693	−2.7
0.4162	0.5838	0.5157	0.5113	−0.9
0.5682	0.4318	0.5366	0.5399	0.6
0.6716	0.3284	0.7190	0.7414	3.1
0.7582	0.2418	0.8690	0.8893	2.3
0.8686	0.1314	1.1120	1.1767	5.8
0.9636	0.0364	1.6350	1.5702	−3.9
0.0372	0.0000	0.4040	0.4091	1.3
0.1351	0.0000	0.4189	0.4262	1.7
0.2152	0.0000	0.4349	0.4449	2.3
0.3546	0.0000	0.4818	0.4914	2.0
0.4060	0.0000	0.5063	0.5147	1.7
0.5723	0.0000	0.6309	0.6263	−0.7
0.6165	0.0000	0.6778	0.6429	−5.1
0.7122	0.0000	0.8201	0.7929	−3.3
0.8948	0.0000	1.2618	1.2413	−1.6
0.9290	0.0000	1.4136	1.3815	2.3
0.0000	0.0987	0.3930	0.3968	1.0
0.0000	0.1581	0.3895	0.3932	−0.9
0.0000	0.2246	0.3854	0.3898	1.1
0.0000	0.3465	0.3884	0.3856	−0.7
0.0000	0.4906	0.3813	0.3841	0.7
0.0000	0.5977	0.3943	0.3856	−2.2
0.0000	0.6444	0.3904	0.3871	−0.8
0.0000	0.7507	0.3908	0.3924	0.4
0.0000	0.8015	0.3970	0.3959	0.3
0.0000	0.9502	0.4100	0.4110	0.2

Table 5. Binary interaction parameters (k_{ij}) and calculated (AAD%) in kinematic viscosity by using M_4 equation of state for the binary mixtures at different temperatures (K).

	298.15 K		308.15 K		313.15 K	
Mixture	k_{ij}	AAD%	k_{ij}	AAD%	k_{ij}	AAD%
2-Propanol (1) + ethyl acetate (2)	−0.115	3.2	−0.0114	3.1	−0.110	2.4
2-Propanol (1) + *n*-hexane (3)	−0.125	3.1	−0.125	1.9	−0.124	2.2
Ethyl acetate (2) + *n*-hexane (3)	−0.019	0.4	−0.019	0.4	−0.018	0.83

Table 6. Calculated (AAD%) in kinematic viscosity by using M_4 equation of state for the ternary mixture of [2-propanol (1) + ethyl acetate (2) + *n*-hexane (3)] at different temperatures (K).

298.15 K	308.15 K	313.15 K
AAD%		
3.5	1.9	1.6

of state (a and b) were calculated by the simple one-parameter van der Waals one-fluid (vdW-1) mixing rule. The binary interaction parameters were used for viscosity calculations of the studied ternary mixture.

Comparison of the calculated results with the experimental data indicates the applicability of the used model based on equation of state approach for predicting the viscosities of binary and ternary mixtures.

List of symbols

a	attractive parameter of M_4 equation of state
b	repulsive parameter of M_4 equation of state
AAD	average absolute deviation
$G^{\#E}$	excess Gibbs energy of viscous flow in equations (1) and (3)
G^{E}	excess Gibbs free energy in equation (4)
K_{ij}	binary interaction parameters
n_1, n_2	constants of M_4 equation of state
n_i	number of moles component i
N	number of experimental points
P	pressure
R	Universal gas constant
V, V^*	molar volume
T	temperature
x_i	liquid mole fraction of the ith component
Z	compressibility factor

Greek letters

η	viscosity
η_i^*	viscosity of pure component i
ϕ_i^*	fugacity coefficient of pure component i
ϕ_i	fugacity coefficient of component i in the mixture
ω	acentric factor
ν	kinematic viscosity
ρ	density

Subscripts

c	critical property
id	ideal
i,j	components
mix	mixture
r	reduced property
calc.	calculated value
exp.	experimental value

Superscripts

*	pure component

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Appendix A: Fugacity coefficient expression derived from the M_4 equation of state

The M_4 equation of state is in the following form [13]:

$$P = \frac{RT}{V}\left(\frac{V+\alpha b}{V-b}\right) - \frac{a}{T^{1/2}V(V+2\alpha b)} \tag{A1}$$

The parameters a and b of this equation is expressed as:

$$a = a_c\left[1 + m\left(1 - T_r^{0.5}\right)\right]^2 \tag{A2}$$

$$b = b_c\left[1 + n_1\left(1 - T_r^{0.5}\right) + n_2\left(1 - T_r^{0.75}\right)\right]^2 \quad \text{for } T_r < 1 \tag{A3}$$

where a_c and b_c are the critical parameters of M_4 equation of state expressed in terms of critical temperature T_c and pressure P_c:

$$a_c = 0.47312\left(\frac{R^2 T_C^{2.5}}{P_C}\right) \tag{A4}$$

$$b_c = 0.04616\left(\frac{RT_C}{P_C}\right) \tag{A5}$$

and

$$m = 0.32(1 + 2\omega) \tag{A6}$$

$$n_1 = 3.270572 - 6.4127\omega + 10.6821\omega^2 \tag{A7}$$

$$n_2 = -1.72192 + 3.85288\omega - 7.202286\omega^2 \tag{A8}$$

where ω is the acentric factor.

The fugacity coefficient of component *i* can be derived by using the following well-known expression [14]:

$$\ln\phi_i = \frac{1}{RT}\int_V^\infty \left[\left(\frac{\partial P}{\partial n_i}\right)_{T,V,n_j} - \frac{RT}{V}\right]\mathrm{d}V - \ln Z \tag{A9}$$

where Z is the compressibility factor.

Therefore, by using equations (A1)–(A8) in equation (A9) along the vdW-1 mixing rules (equations (13) and (14) in the text) the following equation for fugacity coefficient of component *i* for M_4 equation of state will be obtained as:

$$\ln\phi_i = \frac{1}{2RT^{1.5}\alpha b}\left[a\left(\frac{b_i}{b}\right) - 2\sum_{j=1}^{N} x_j a_{ij}\right]\ln\frac{V+2\alpha b}{V} + (Z-1)\left(\frac{b_i}{b}\right) - \ln\left[Z\left(\frac{V-b}{V}\right)^{\alpha+1}\right] \tag{A10}$$