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Theoretical and experimental study of molecular interaction between Propylene glycol and Ether alcohols

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ABSTRACT

This study investigates the thermophysical properties of binary liquid mixtures of propylene glycol (PG) with ether alcohols-propylene glycol monopropyl ether (2-PE) and ethylene glycol monobutyl ether (2-BE)-across the entire composition range at temperatures T= (298.15 - 323.15) K. Viscosity measurements were performed at T= (298.15 - 308.15) K. From the experimental data, excess properties such as molar volume, isentropic compressibility, speed of sound, isobaric thermal expansion coefficient, and deviation in viscosity were calculated. Partial molar properties and their excess values, including those at infinite dilution, were also derived. The excess properties were correlated using the Redlich-Kister polynomial, and the results were analysed using the Prigogine-Flory-Patterson theory to explore intermolecular interactions. Viscosity correlations were carried out using empirical and semi-empirical models, while density was modelled using the perturbed chain statistical associating fluid theory (PC-SAFT), accounting for hydrogen bonding effects. The speed of sound was predicted using Schaaff's collision factor theory (SCFT) and Nomoto's relation (NR), with density data from PC-SAFT as input. Viscosity modelling employed free volume theory (FVT) as a fitted approach. The findings provide insights into the thermophysical behaviour of these mixtures and the role of intermolecular interactions.

1. Introduction

Flow, mass transfer, and heat transfer calculations play a crucial role in the design and optimization of various chemical and industrial processes such as in chemical, textile, leather, pharmaceutical, and nuclear industries [1]. Non-aqueous binary liquid mixes' physicochemical properties are essential in theoretical and practical research. Investigating the thermodynamic behaviour of non-ideal binary mixtures provides valuable insights into molecular interactions and structural organisation within liquid systems. Under the assumption of negligible absorption of low-frequency, low-amplitude sound waves, the speed of sound can be treated as a thermodynamic property [2]. We report here the results of six temperature-dependent volumetric and ultrasonic studies on binary mixtures of Propylene glycol (PG) with Ether alcohols (2-propoxyethanol (2-PE) and 2-Butoxyethanol (2-BE). These studies extended our ongoing theoretical and experimental investigations into the physicochemical properties of binary liquid mixtures of non-aqueous [3–6].

Propanediols exhibit polarity and can form hydrogen bonds between and within molecules [7]. This hydrogen bonding is more pronounced in glycols than in alcohols with only one hydroxylic group. Propylene glycol (PG) has numerous applications in various industries. It is commonly used as an antifreeze, coolant, plasticiser, pharmaceutical ingredient, cosmetic additive, and food additive. Additionally, it is utilised in the tobacco and petroleum industry as a heat transfer fluid and in hydraulic fluids [8–10]. The dielectric constant of ~~1,2-propanediol, or~~ propylene glycol, is approximately 32 at 293.15 K. The relatively high dielectric constant of propylene glycol contributes to its usefulness in various applications, such as in the production of capacitors and as a dielectric solvent. 2-PE and 2-BE belong to a class of compounds known as glycol ethers. These compounds have gained significant interest due to their practical applications, mainly as additives in petrol. Oxygenated molecules like glycol ethers are being increasingly used in petrol due to their ability to improve octane levels and reduce pollution [11,12]. They have a remarkable ability to dissolve various substances, making them highly valuable in multiple formulations like paints, coatings, and

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Table 1
Details of studied compounds, CAS number, source, purification method, purity and analysis method.

Chemical name	CAS number	Source	Purification method	Initial Mass fraction purity (stated by the supplier)	Analysis method	Final Mass fraction purity	Water Content (ppm)*
1,2-propanediol	57-55-6	Sigma Aldrich	molecular sieves treatment, degassing in a vacuum	>0.99	GC	>0.992	80
2-propoxyethnol	2807-30-9	Sigma Aldrich	molecular sieves treatment, degassing in a vacuum	≥0.99	GC	>0.996	98
2-butoxyethanol	111-76-2	Sigma Aldrich	molecular sieves treatment, degassing in a vacuum	≥0.99	GC	>0.996	103

GC= Gas chromatography, *Karl fisher Titration.

cleaning products. The combination of blended mixtures has vast applications in industry as a solvent in coatings and paints to enhance solvency and improve formulation properties, in cleaning products, in the formulation of inks for printing, serve as effective solvents or co-solvents, used to improve performance characteristics such as drying time, film formation, and gloss, as versatile reagents in the synthesis of other chemicals, providing a balance of reactivity and solubility, in personal care products, such as lotions or creams.

Along with the applications mentioned above, other applications of these binary mixtures of Propylene glycol (PG) with Ether alcohols exhibit properties that make them valuable in the petroleum industry and second-generation fluids. The applications of this mixture are diverse, ranging from solvency and hydrophobicity in cleaning agents to providing thermal stability and viscosity control in advanced fluid formulations.

So, based on the applications, we have chosen these chemicals, and a systematic investigation of the binary mixture has been done, but data is not available. Systematic investigation of the physicochemical properties of Propylene glycol (PG) with some molecular organic solvents, including water, alkanols, hydrocarbons, and Ionic liquids, has been reported [13–24]. Still, the data with α,ω-alkanediol with solutes are scanty.

In the present paper, the physical properties of density and speed of sound of pure liquids and their blends have been measured at T=298.15-323.15 K at atmospheric pressure with equal intervals of temperature (5°C) and mole fraction (0.1). From the measured values, excess molar volume (V_m^E), excess isentropic compressibility ($K_{s,m}^E$), excess molar isentropic compressibility ($K_{s,m}^E$), excess speed of sound (u^E), excess isobaric thermal expansivity (α_p^E), and fitted with the R-K polynomial equation. Using R-K coefficients, excess partial molar volume and compressibility have been measured, as well as excess partial molar volume and compressibility at infinite dilution. The liquid density for the 1,2-propanediol + 2-PE and 1,2-propanediol + 2-BE mixtures was calculated through the application of the perturbed chain statistical associating fluid theory equation of state (PC-SAFT EoS) [25,26] as a predictive approach. Schaaff's collision factor theory (SCFT) [27] and Nomoto's relation (NR) [28], both coupled to the PC-SAFT EoS, were used to compute the speed of sound as the predictive approach. Finally, the model called free volume theory (FVT) [29–31] was coupled to PC-SAFT EoS to model the viscosity of the mixtures.

2. Experimental

2.1. Material

Propylene glycol and Ether alcohols supplied by Sigma-Aldrich with a purity of 0.99 in mass fraction were used in the study and were purified by the methods described in the literature [16,32]. Karl Fischer titrator (Mtrohm, 890 Titrando) was used to test the solute and solvent water content [33]. Before use, all chemicals were stored over 0.4 nm molecular sieves for 72 hrs to remove any residual water, and subsequently degassed by ultrasonic agitation at atmospheric pressure (0.1 MPa). The GC confirmed that the compounds were over 99% pure after purification. We compared the Pure liquid density and sound speed of 2-PE and 2-BE with the literature and provided in the *supplementary information* Tables 1S & 2S. A graphical comparison was made in the supplementary information as Fig. 1S-4S. The density, ultrasonic velocity and viscosity of PG were taken from our recent paper [64]. Pure and binary liquids were stored in amber dark bottles over activated 0.4 nm molecular sieves [34,35]. In Table 1, suppliers and the purity of the liquids were reported. Viscosity 2-BE and 2-PE have been compared with the literature and graphically shown in *Supplementary Information as* Table 3S (Fig.5S) with AAD. The viscosity of PG + 2-BE was fitted with a constrained Jouyban-Acree-type Polynomial equation and given as Table 4S in the Supplementary information.

Table 2
Densities, ρ, and speeds of sound, u, as a function of mole fraction of 1,2-PD at T = (298.15 – 323.15) K and at pressure 0.1 MPa.

x_1	ρ/kg.m^{-3} T = 298.15 K	u/m.s^{-1}	ρ/kg.m^{-3} T = 303.15 K	u/m.s^{-1}	ρ/kg.m^{-3} T = 308.15 K	u/m.s^{-1}	ρ/kg.m^{-3} T = 313.15 K	u/m.s^{-1}	ρ/kg.m^{-3} T = 318.15 K	u/m.s^{-1}	ρ/kg.m^{-3} T = 323.15 K	u/m.s^{-1}
1,2-PD + 2-PE												
0.0000	909.11	1300.9 [5]	904.71	1283.7 [5]	900.27	1266.4 [6]	895.80	1249.2 [5]	891.29	1231.9 [5]	886.89	1215.0 [5]
0.1127	923.03	1324.6	918.71	1307.7	914.35	1290.8	909.96	1273.9	905.53	1257.1	901.19	1240.4
0.1957	933.29	1342.0	929.03	1325.4	924.72	1308.8	920.39	1292.2	916.02	1275.6	911.73	1259.1
0.2980	945.93	1363.5	941.74	1347.3	937.50	1331.0	933.24	1314.7	928.94	1298.4	924.71	1282.2
0.3832	956.44	1381.4	952.32	1365.5	948.14	1349.4	943.94	1333.4	939.70	1317.4	935.52	1301.5
0.4881	969.40	1403.4	965.35	1387.9	961.24	1372.2	957.11	1356.5	952.95	1340.8	948.82	1325.1
0.6047	983.81	1427.9	979.84	1412.8	975.82	1397.5	971.77	1382.1	967.69	1366.8	963.63	1351.5
0.6937	994.80	1446.6	990.90	1431.8	986.93	1416.7	982.95	1401.7	978.93	1386.6	974.92	1371.6
0.8055	1008.62	1470.1	1004.79	1455.6	1000.90	1441.0	997.00	1426.3	993.06	1411.5	989.11	1396.8
0.8532	1014.50	1480.1	1010.71	1465.8	1006.86	1451.3	1002.99	1436.8	999.08	1422.2	995.16	1407.6
1.0000	1032.64 [4]	1511.0 [64]	1028.95 [4]	1497.2 [64]	1025.20 [4]	1483.1 [64]	1021.43 [4]	1469.0 [64]	1017.63 [4]	1454.9 [64]	1013.79 [4]	1440.7 [64]
1,2-PD + 2-BE												
0.0000	897.05	1306.5	892.63	1290.3 [6]	888.19	1274.1 [6]	883.73	1257.9 [6]	879.33	1241.7 [6]	874.85	1225.5
0.1080	911.69	1328.6	907.35	1312.6	902.98	1296.7	898.59	1280.7	894.26	1264.7	889.85	1248.7
0.1968	923.73	1346.7	919.46	1331.0	915.15	1315.2	910.83	1299.4	906.55	1283.7	902.19	1267.9
0.3098	939.05	1369.8	934.86	1354.4	930.63	1338.8	926.39	1323.3	922.17	1307.8	917.89	1292.2
0.3995	951.22	1388.2	947.09	1372.9	942.93	1357.6	938.74	1342.2	934.58	1326.9	930.36	1311.5
0.5080	965.93	1410.4	961.88	1395.4	957.79	1380.3	953.68	1365.2	949.59	1350.0	945.43	1334.8
0.5969	977.98	1428.5	974.00	1413.8	969.97	1398.9	965.92	1383.9	961.88	1369.0	957.78	1354.0
0.7075	992.98	1451.2	989.08	1436.7	985.13	1422.0	981.16	1407.3	977.18	1392.6	973.15	1377.8
0.7910	1004.30	1468.2	1000.46	1453.9	996.57	1439.4	992.65	1424.9	988.73	1410.4	984.75	1395.8
0.8983	1018.84	1490.2	1015.08	1476.1	1011.26	1461.9	1007.42	1447.5	1003.56	1433.2	999.65	1418.8
1.0000	1032.64 [64]	1511.0 [64]	1028.95 [64]	1497.2 [64]	1025.20 [64]	1483.1 [64]	1021.43 [64]	1469.0 [64]	1017.63 [64]	1454.9 [64]	1013.79 [64]	1440.7 [64]

Standard uncertainties u are u(T) = ± 0.01 K, u(x) = ±1.0 × 10-3, u(ρ) = ±0.9 kg•m-3, u(u) = ± 0.7 m•s-1 and u(p) = ±1.0 kPa.

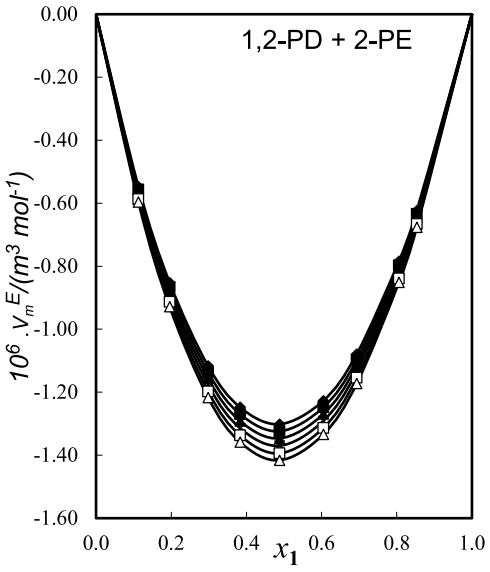

Fig. 1. Plots of excess molar volume, V_m^E vs. mole fraction, x1 of 1,2-PD for 1,2-PD + 2-PE binary mixtures at temperatures, T/K = 298.15, ; At T/K = 303.15, ■; T/K = 308.15, ▲; T/K = 313.15, ×; T/K = 318.15, ; T/K = 323.15, Δ. The points represent experimental values, and the lines represent values calculated from Eq. (13).

2.2. Apparatus and procedure

The pure liquids and the binary mixture densities (ρ) and Speed of Sound (u) have been measured with the DSA 5000 M instrument from Anton Paar, Austria. This device offers a reproducibility of ±1 × 10^3 kg/m^3 for density measurements and ±1 × 10^2 *m/s* for sound velocity, operating at a frequency of 3 *MHz*. The densimeter is continuously calibrated at atmospheric pressure using dry air and deionised water. After each use, the instrument is cleaned with triple-distilled water followed by anhydrous ethanol. The standard uncertainties for temperature, density, and speed of sound have been estimated at ±0.01 *K*, ±0.9 *kg/m^3*, and ±0.7 *m/s*, respectively, at a confidence level, $k = 1$.

A Ubbelohde-type suspended level viscometer has been used to measure the viscosity of the pure liquids and the mixtures, calibrating it with triply distilled water. To maintain the temperature stability of the test liquid, the viscometer was kept in a thermostatic water bath for a period of 30 min. The flow times were determined in triplicate on a digital stopwatch with an accuracy of ± 0.01*s* , and the viscosity values could be read with a repeatability of ±5·0 × 10^{-7} *N·s·m^{-2}*. An electronically controlled thermostatic water bath (Model: ME 31A, JULABO, Germany) was used to keep the temperature of the measurements within an uncertainty of ±0.01 *K*. The relative uncertainty of viscosity $u_r(\eta)$=2%.

3. Theory

The experimental density (ρ) and sound velocity (u) of pure and its mixtures having Propylene glycol with Ether alcohols in the temperature range (298.15-323.15) K are presented in Table 2. The experimental viscosity of pure and its binary mixtures at 298.15 & 303.15 is presented in Table 4. The graphical comparison of density, sound velocity and viscosity in the form of ARD (Average relative deviation) is given in Table 1S-3S & Fig. 1S-5S in the *supplementary information.*

From the experimental densities, the excess molar volumes, V_m^E have been computed by the relation

$$V_{\mathrm{m}}^{\mathrm{E}} = [(x_1M_1 + x_2M_2)/\rho_{\mathrm{m}}] - [(x_1M_1/\rho_1) + (x_2M_2/\rho_2)] \quad (1)$$

where x_1 and x_2 are the mole fractions, M_1 and M_2 the molar masses of the PG and 2-BE/2-PE respectively, and ρ_1, ρ_2 and ρ_{m} are the densities of the pure components of Propylene glycol (PG) with Ether alcohols and its binary mixtures, respectively.

The isentropic compressibilities, κ_{s} of the pure components and their binary mixtures, measured by the equation [36]

Table 3
Excess molar volume (V_m^E), excess isentropic compressibility (κ_s^E), excess molar isentropic compressibility ($K_{s,m}^E$), excess speed of sound (u^E) and excess isobaric expansivity (α_p^E) as a function of mole fraction, x_1 of 1,2-propanediol for 2-EE/2-BE + 1,2-propanediol at the temperatures T = (298.15 to 323.15) K at pressure p = 0.1 MPa.

x_1	V_m^E 10^6 $m^3 \bullet mol^{-1}$	κ_s^E 10^{10} $m^2 \bullet N^{-1}$	$K_{s,m}^E$ 10^{14} $m^5 \bullet N^{-1} \bullet mol^{-1}$	u^E 10^2 m.s^{-1}	α_p^E 10^4 K^{-1}
2-propoxyethanol + 1,2-propanediol					
298.15 K					
0.1127	-0.5470	-0.1721	-0.2230	0.1482	-4.1963
0.1957	-0.8518	-0.2743	-0.3430	0.2463	-7.2455
0.2980	-1.1168	-0.3709	-0.4432	0.3514	-10.4108
0.3832	-1.2478	-0.4258	-0.4895	0.4227	-12.3849
0.4881	-1.3015	-0.4604	-0.5038	0.4855	-13.8932
0.6047	-1.2269	-0.4532	-0.4683	0.5136	-14.2022
0.6937	-1.0785	-0.4128	-0.4076	0.4965	-13.2439
0.8055	-0.7843	-0.3149	-0.2930	0.4111	-10.2082
0.8532	-0.6235	-0.2558	-0.2319	0.3469	-8.2279
303.15 K					
0.1127	-0.5567	-0.1829	-0.2375	0.1513	-4.2518
0.1957	-0.8668	-0.2913	-0.3650	0.2516	-7.3369
0.2980	-1.1363	-0.3936	-0.4713	0.3590	-10.5411
0.3832	-1.2695	-0.4518	-0.5203	0.4320	-12.5417
0.4881	-1.3239	-0.4882	-0.5351	0.4965	-14.0728
0.6047	-1.2478	-0.4803	-0.4971	0.5257	-14.3902
0.6937	-1.0968	-0.4373	-0.4325	0.5086	-13.4233
0.8055	-0.7975	-0.3334	-0.3107	0.4217	-10.3533
0.8532	-0.6339	-0.2707	-0.2458	0.3560	-8.3490
308.15 K					
0.1127	-0.5665	-0.1933	-0.2518	0.1534	-4.3073
0.1957	-0.8820	-0.3078	-0.3867	0.2551	-7.4284
0.2980	-1.1561	-0.4155	-0.4990	0.3642	-10.6715
0.3832	-1.2914	-0.4766	-0.5504	0.4384	-12.6986
0.4881	-1.3466	-0.5146	-0.5656	0.5040	-14.2526
0.6047	-1.2690	-0.5058	-0.5249	0.5340	-14.5785
0.6937	-1.1153	-0.4602	-0.4563	0.5169	-13.6028
0.8055	-0.8108	-0.3506	-0.3275	0.4289	-10.4987
0.8532	-0.6445	-0.2847	-0.2590	0.3623	-8.4703
313.15 K					
0.1127	-0.5766	-0.2046	-0.2673	0.1556	-4.3644
0.1957	-0.8976	-0.3255	-0.4102	0.2589	-7.5220
0.2980	-1.1764	-0.4391	-0.5288	0.3696	-10.8041
0.3832	-1.3140	-0.5033	-0.5829	0.4451	-12.8577
0.4881	-1.3699	-0.5431	-0.5985	0.5120	-14.4340
0.6047	-1.2908	-0.5334	-0.5549	0.5428	-14.7676
0.6937	-1.1344	-0.4850	-0.4821	0.5257	-13.7826
0.8055	-0.8246	-0.3692	-0.3457	0.4366	-10.6438
0.8532	-0.6554	-0.2997	-0.2733	0.3690	-8.5912
318.15 K					
0.1127	-0.5870	-0.2166	-0.2839	0.1578	-4.4226
0.1957	-0.9137	-0.3444	-0.4354	0.2626	-7.6185
0.2980	-1.1974	-0.4643	-0.5608	0.3752	-10.9423
0.3832	-1.3372	-0.5319	-0.6178	0.4520	-13.0247
x_1	V_m^E 10^6 $m^3 \bullet mol^{-1}$	κ_s^E 10^{10} $m^2 \bullet N^{-1}$	$K_{s,m}^E$ 10^{14} $m^5 \bullet N^{-1} \bullet mol^{-1}$	u^E 10^2 $m.s^{-1}$	α_p^E 10^4 K^{-1}
0.4881	-1.3940	-0.5735	-0.6338	0.5202	-14.6261
0.6047	-1.3133	-0.5629	-0.5872	0.5519	-14.9695
0.6937	-1.1540	-0.5116	-0.5098	0.5350	-13.9757
0.8055	-0.8387	-0.3893	-0.3653	0.4448	-10.8005
0.8532	-0.6666	-0.3159	-0.2887	0.3761	-8.7221
323.15 K					
0.1127	-0.5966	-0.2283	-0.3002	0.1593	-4.4741
0.1957	-0.9286	-0.3628	-0.4602	0.2652	-7.7033
0.2980	-1.2167	-0.4887	-0.5922	0.3789	-11.0633
0.3832	-1.3587	-0.5594	-0.6518	0.4565	-13.1705
0.4881	-1.4161	-0.6027	-0.6681	0.5256	-14.7936
0.6047	-1.3340	-0.5910	-0.6184	0.5580	-15.1454
0.6937	-1.1720	-0.5368	-0.5365	0.5411	-14.1437
0.8055	-0.8517	-0.4082	-0.3841	0.4503	-10.9370
0.8532	-0.6769	-0.3311	-0.3034	0.3809	-8.8362
2-butoxyethanol + 1,2-propanediol					
298.15 K					
0.1080	-0.8315	-0.1894	-0.2894	0.1544	-5.6764
0.1968	-1.3470	-0.3177	-0.4626	0.2706	-10.2068
0.3098	-1.7925	-0.4433	-0.6060	0.4004	-15.1205
0.3995	-1.9854	-0.5115	-0.6635	0.4852	-18.0912
0.5080	-2.0369	-0.5535	-0.6720	0.5594	-20.3534
0.5969	-1.9367	-0.5517	-0.6327	0.5897	-20.8950
0.7075	-1.6405	-0.4981	-0.5300	0.5747	-19.4496
0.7910	-1.2958	-0.4145	-0.4155	0.5101	-16.4000
0.8983	-0.7062	-0.2429	-0.2245	0.3285	-9.5383
303.15 K					
0.1080	-0.8456	-0.1997	-0.3059	0.1567	-5.7435
0.1968	-1.3697	-0.3348	-0.4888	0.2747	-10.3247
0.3098	-1.8223	-0.4670	-0.6400	0.4066	-15.2963
0.3995	-2.0182	-0.5386	-0.7003	0.4929	-18.3054
0.5080	-2.0703	-0.5826	-0.7089	0.5685	-20.6004
0.5969	-1.9682	-0.5805	-0.6671	0.5996	-21.1537
0.7075	-1.6669	-0.5239	-0.5586	0.5849	-19.6974
0.7910	-1.3165	-0.4358	-0.4377	0.5195	-16.6155
0.8983	-0.7174	-0.2553	-0.2364	0.3350	-9.6721
308.15 K					
0.1080	-0.8597	-0.2096	-0.3223	0.1580	-5.8096
0.1968	-1.3923	-0.3512	-0.5146	0.2771	-10.4406
0.3098	-1.8521	-0.4895	-0.6731	0.4102	-15.4692
0.3995	-2.0510	-0.5643	-0.7362	0.4974	-18.5160
0.5080	-2.1036	-0.6099	-0.7445	0.5738	-20.8433
0.5969	-1.9997	-0.6074	-0.7002	0.6054	-21.4082
0.7075	-1.6933	-0.5478	-0.5858	0.5908	-19.9411
0.7910	-1.3372	-0.4554	-0.4588	0.5250	-16.8274
0.8983	-0.7286	-0.2667	-0.2476	0.3388	-9.8037
313.15 K					
0.1080	-0.8741	-0.2203	-0.3398	0.1595	-5.8765
0.1968	-1.4155	-0.3688	-0.5422	0.2796	-10.5576
0.3098	-1.8826	-0.5136	-0.7087	0.4141	-15.6431
0.3995	-2.0845	-0.5917	-0.7745	0.5021	-18.7273
x_1	V_m^E 10^6 $m^3 \bullet mol^{-1}$	κ_s^E 10^{10} $m^2 \bullet N^{-1}$	$K_{s,m}^E$ 10^{14} $m^5 \bullet N^{-1} \bullet mol^{-1}$	u^E 10^2 $m.s^{-1}$	α_p^E 10^4 K^{-1}
0.5080	-2.1377	-0.6391	-0.7827	0.5795	-21.0863
0.5969	-2.0318	-0.6362	-0.7357	0.6116	-21.6621
0.7075	-1.7203	-0.5733	-0.6150	0.5971	-20.1837
0.7910	-1.3584	-0.4765	-0.4813	0.5309	-17.0379
0.8983	-0.7400	-0.2788	-0.2596	0.3430	-9.9340
318.15 K					
0.1080	-0.8880	-0.2315	-0.3583	0.1609	-5.9397
0.1968	-1.4378	-0.3874	-0.5715	0.2823	-10.6689
0.3098	-1.9120	-0.5393	-0.7464	0.4181	-15.8098
0.3995	-2.1168	-0.6209	-0.8153	0.5072	-18.9311
0.5080	-2.1705	-0.6704	-0.8233	0.5857	-21.3225
0.5969	-2.0628	-0.6670	-0.7735	0.6184	-21.9106
0.7075	-1.7463	-0.6008	-0.6462	0.6041	-20.4229
0.7910	-1.3788	-0.4992	-0.5055	0.5375	-17.2468
0.8983	-0.7510	-0.2920	-0.2725	0.3477	-10.0645
323.15 K					
0.1080	-0.9026	-0.2426	-0.3771	0.1617	-6.0059
0.1968	-1.4613	-0.4057	-0.6009	0.2836	-10.7851
0.3098	-1.9429	-0.5642	-0.7840	0.4202	-15.9832
0.3995	-2.1507	-0.6492	-0.8557	0.5098	-19.1425
0.5080	-2.2050	-0.7003	-0.8634	0.5887	-21.5666
0.5969	-2.0953	-0.6964	-0.8105	0.6218	-22.1667
0.7075	-1.7736	-0.6268	-0.6765	0.6077	-20.6688
0.7910	-1.4002	-0.5204	-0.5289	0.5409	-17.4610
0.8983	-0.7626	-0.3042	-0.2848	0.3501	-10.1980

Standard uncertainties u are as follows: u(x) = 1 × 10-3, u(V_m^E)=±0.005•10-6 m3•mol-1, u(κ_s^E) = ±0.05•1010 m2•N-1, u($K_{s,m}^E$) = ±0.004•1014 m5•N-1•mol-1, u(u^E) = ±0.05•1010 102 m.s-1, u(α_p^E) = ±0.003 kK-1, u(p) = ± 1.0 kPa.

$$\kappa_s = -V_m(\partial V_m/\partial P)_s = (\rho u^2)^{-1} = V_m(Mu^2)^{-1} \quad (2)$$

The excess and excess molar isentropic compressibilities are calculated by using the relation [37,38] proposed by Benson and Kiyohara.

$$\kappa_s^E = \kappa_s - \kappa_s^{id} \quad (3)$$

$$K_{S,M}^E = K_{S,M} - K_{S,M}^{id} \quad (4)$$

Table 4
Viscosity, η/(mPa•s) and excess deviation of Viscosity ($\Delta\eta$), as a function of mole fraction of 1,2-PD for 2-BE/PE + 1,2-propanediol at the temperatures T = (298.15 to 308.15) K at pressure p = 0.1 MPa.

	298.15		303.15	
x_1	η	$\Delta\eta$	η	$\Delta\eta$
2-PE+1,2-PD				
0.0000	2.35	0.00	2.12	0.00
0.1127	3.62	-3.38	3.12	-2.65
0.1957	4.73	-5.69	4.05	-4.40
0.2980	6.38	-8.25	5.39	-6.37
0.3832	8.10	-10.03	6.71	-7.80
0.4881	10.82	-11.64	8.73	-9.17
0.6047	14.91	-12.35	11.74	-9.94
0.6937	19.05	-11.88	14.82	-9.73
0.8055	25.87	-9.66	20.07	-8.09
0.8532	29.45	-8.05	22.90	-6.80
1.0000	43.55[64]	0.00	34.45[64]	0.00
2-BE+1,2-PD				
0.0000	2.79	0.00	2.4	0.00
0.1080	3.73	-3.45	2.79	-3.07
0.1968	4.75	-6.06	3.37	-5.34
0.3098	6.46	-8.95	4.54	-7.79
0.3995	8.26	-10.81	5.97	-9.23
0.5080	11.13	-12.37	8.50	-10.18
0.5969	14.21	-12.90	11.44	-10.09
0.7075	19.30	-12.33	16.39	-8.69
0.7910	24.33	-10.70	21.08	-6.67
0.8983	32.79	-6.61	27.96	-3.23
1.0000	43.55[64]	0.00	34.45 [64]	0.00

Standard uncertainties u are u(T) = ± 0.01 K, $u(x_1)$ = ± 1 × 10^{-3} and $u_r(\eta)$ = ± 2% *MPa•s*. $u(p)$ = ± 1.0 *kPa*.

Excess speed of sound, u^E in binary mixtures, can be calculated using the expression [36,39]

$$u^{\mathrm{E}} = u - u^{\mathrm{id}} = u - \left(\rho^{\mathrm{id}}\kappa_s^{\mathrm{id}}\right)^{-1/2} \tag{5}$$

Excess isobaric thermal expansivity α_p^E, can be computed by the formulae [40]

$$\alpha_p^E \Big/ \left(K^{-1}\right) = \alpha_p - \alpha_p^{id} = \left(\partial V_m/\partial T\right)_p \Big/ V_m - \sum_{i=1}^{2} \phi_i \alpha_{p,i}^{*} \tag{6}$$

The viscosity (η) and deviation in viscosity ($\Delta\eta$) were given in Table 4. Deviation in viscosity can be calculated using the relation

$$\Delta\eta = \eta - (x_1\eta_1 + x_2\eta_2) \tag{7}$$

In Tables 3 and 4, the values of V_m^E, κ_s^E, $K_{s,m}^E$, u^E, α_p^E, and $\Delta\eta$ have been given as a function of Propylene glycol (x_1) at investigated temperature

The Redlich-Kister [41] polynomial equation is used to fit the values of the excess properties for the mixtures, and the ideal number of A_i coefficients has been found using the F-test.

$$Y^E = x_1 x_2 \sum_{k=0}^{p} A_k (2x_1 - 1)^i \tag{8}$$

where Y^{E} is V_m^E, κ_s^E, $K_{s,m}^E$, u^{E}, andα_p^E.

The coefficients, denoted as A_k, have been determined utilising the least squares method, where all data points were assigned equal weight. The standard deviations of the fit, represented by σ, were computed using a specific relationship.

$$\sigma = \left[\sum \left(Y_{\mathrm{Calc.}}^{\mathrm{E}} - Y_{\mathrm{Expt.}}^{\mathrm{E}}\right)^2 \Big/ (m - i)\right]^{1/2} \tag{9}$$

Table 5 contains the list of A_k coefficients, and the accompanying standard deviations, σ of the mixtures.

The variations of V_m^E, κ_s^E, $K_{s,m}^E$, u^E, α_p^E and $\Delta\eta$with mole fraction, x_1,

Table 5
Coefficients A_j of Eq. (13) along with standard deviations σ of binary mixture properties.

Parameter	T/K	A_0	A_1	A_2	Std Dev	Std Err
1,2-PD +2-PE						
$V_{m,1}^E/10^6\ m^3mol^{-}$	298.15	-5.2010	0.3316	-0.0219	0.468	6.898E-05
	303.15	-5.2904	0.3408	-0.0225	0.476	5.714E-05
	308.15	-5.3810	0.3502	-0.0232	0.484	7.534E-05
	313.15	-5.4742	0.3594	-0.0243	0.493	6.332E-05
	318.15	-5.5703	0.3694	-0.0246	0.501	7.788E-05
	323.15	-5.6587	0.3789	-0.0254	0.509	8.115E-05
$\kappa_s^E/10^{10}\ m^2.N^{-1}$	298.15	-1.8477	-0.2185	-0.0762	0.167	2.100E-04
	303.15	-1.9592	-0.2267	-0.0802	0.177	1.923E-04
	308.15	-2.0649	-0.2311	-0.0845	0.187	2.385E-04
	313.15	-2.1790	-0.2362	-0.0887	0.197	2.260E-04
	318.15	-2.3009	-0.2426	-0.0945	0.208	2.512E-04
	323.15	-2.4178	-0.2455	-0.0993	0.219	2.715E-04
$K_{s,m}^E/10^{14}\ m^5.N^{-1}.mol^{-1}$	298.15	-2.0101	0.2528	-0.0399	0.181	4.955E-05
	303.15	-2.1350	0.2749	-0.0441	0.193	6.071E-05
	308.15	-2.2564	0.3001	-0.0475	0.204	5.717E-05
	313.15	-2.3874	0.3271	-0.0523	0.216	7.530E-05
	318.15	-2.5281	0.3557	-0.0574	0.229	8.565E-05
	323.15	-2.6647	0.3864	-0.0627	0.241	9.878E-05
$u^E/10^2\ m.s^{-1}$	298.15	1.9615	0.8611	0.3552	0.189	2.040E-03
	303.15	2.0061	0.8886	0.3709	0.193	2.138E-03
	308.15	2.0367	0.9078	0.3810	0.196	2.221E-03
	313.15	2.0689	0.9284	0.3924	0.199	2.296E-03
	318.15	2.1023	0.9513	0.4049	0.203	2.397E-03
	323.15	2.1242	0.9665	0.4148	0.205	2.460E-03
$\alpha_p^E/10^3\ K^{-1}$	298.15	-55.982	-17.666	-3.349	5.216	7.71E-02
	303.15	-56.708	-17.970	-3.413	5.285	7.81E-02
	308.15	-57.434	-18.275	-3.478	5.354	7.92E-02
	313.15	-58.166	-18.567	-3.542	5.424	8.02E-02
	318.15	-58.942	-18.906	-3.613	5.498	8.14E-02
	323.15	-59.619	-19.198	-3.677	5.563	8.24E-02
$\Delta\eta/mPa.s$	298.15	-47.82	-20.97	-	4.31	1.53E-01
	303.15	-37.02	-19.67	-6.72	3.48	3.58E-03
1,2-PD + 2-BE						
$V_{m,1}^E/10^6\ m^3mol^{-}$	298.15	-8.1588	0.5734	-0.0401	0.754	1.194E-04
	303.15	-8.2925	0.5885	-0.0413	0.766	1.262E-04

(*continued on next page*)

Table 5 (*continued*)

	308.15	-8.4261	0.6034	-0.0426	0.779	1.267E-04
	313.15	-8.5627	0.6190	-0.0442	0.791	1.175E-04
	318.15	-8.6943	0.6339	-0.0456	0.803	1.084E-04
	323.15	-8.8324	0.6498	-0.0476	0.816	1.227E-04
$\kappa_s^E/10^{10}\ m^2.N^{-1}$	298.15	-2.2076	-0.4218	-0.1604	0.217	7.083E-04
	303.15	-2.3238	-0.4393	-0.1682	0.227	7.391E-04
	308.15	-2.4329	-0.4522	-0.1750	0.238	7.836E-04
	313.15	-2.5495	-0.4657	-0.1832	0.249	7.881E-04
	318.15	-2.6743	-0.4823	-0.1917	0.260	8.457E-04
	323.15	-2.7940	-0.4933	-0.1990	0.250	8.568E-04
$K_{s,m}^E/10^{14}\ m^5.N^{-1}.mol^{-1}$	298.15	-2.6940	0.3459	-0.0618	0.263	6.144E-05
	303.15	-2.8420	0.3722	-0.0666	0.277	5.467E-05
	308.15	-2.9851	0.4021	-0.0721	0.291	6.025E-05
	313.15	-3.1384	0.4341	-0.0773	0.306	7.622E-05
	318.15	-3.3016	0.4666	-0.0835	0.321	7.138E-05
	323.15	-3.4623	0.5040	-0.0905	0.221	9.298E-05
$u^E/10^2\ m.s^{-1}$	298.15	2.2172	1.1659	0.5719	0.225	4.343E-03
	303.15	2.2531	1.1923	0.5891	0.227	4.504E-03
	308.15	2.2741	1.2078	0.5989	0.229	4.608E-03
	313.15	2.2964	1.2245	0.6106	0.232	4.731E-03
	318.15	2.3207	1.2444	0.6235	0.233	4.876E-03
	323.15	2.3328	1.2546	0.6311	7.806	4.946E-03
$\alpha_p^E/10^3\ K^{-1}$	298.15	-80.90	-32.00	-8.30	7.903	1.43E-01
	303.15	-81.88	-32.51	-8.44	7.998	1.45E-01
	308.15	-82.85	-33.00	-8.58	8.093	1.47E-01
	313.15	-83.81	-33.48	-8.72	8.187	1.49E-01
	318.15	-84.75	-33.99	-8.87	8.283	1.51E-01
	323.15	-85.72	-34.49	-9.02	0.754	1.53E-01
$\Delta\eta/mPa.s$	298.15	-49.12	-22.40	-7.71	4.58	2.20E-03
	303.15	-40.69	-5.53	10.54	3.62	1.62E-01

along with the smoothed values from Eq. (8) at investigated temperatures, are represented graphically in Figs. 1-8, respectively.

4. Results and discussion

4.1. Excess properties

Upon careful examination of Table 2, it is evident that the experimental density and speed of sound values decrease with increasing temperature along the mole fraction. The excess molar volumes (V_m^E), for the investigated mixtures of PG with ether alcohols (2-PE & 2-BE) at T = 298.15 - 323.15 K is illustrated in Figs. 1 & 2. The comparison of excess molar volumes, V_m^E, for the binary mixtures at T=298.15 K is illustrated

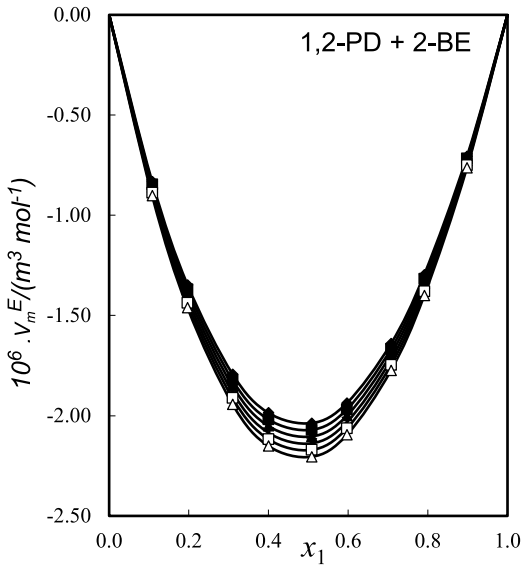

Fig. 2. Plots of excess molar volume, V_m^E vs. mole fraction, x1 of 1,2-PD for 1,2-PD + 2-BE binary mixtures at temperatures, T/K = 298.15; At T/K = 303.15, ■; T/K = 308.15, ▲; T/K = 313.15, ×; T/K = 318.15, □; T/K = 323.15, Δ. The points represent experimental values and the lines represent values calculated from Eq. (13).

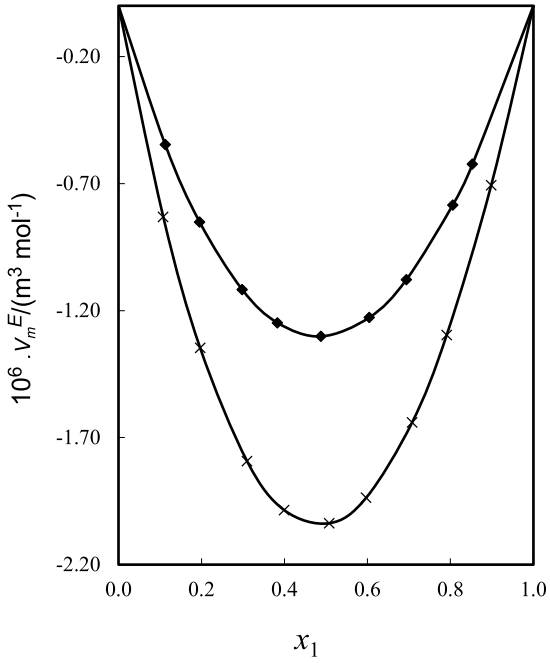

Fig. 3. Variation of excess molar volume (V_m^E) with mole fraction x_1 of 1,2-PD in the binary mixtures of 1,2-PD (1) with alkoxyalkanols (2); (◆), 2-PE; (×), 2-BE at T=298.15 K. The points represent experimental values and solid lines have been drawn from Eq. (13) using the coefficients given in Table 5.

in Fig. 3. It is noteworthy that the V_m^E values have been consistently negative throughout the mole fraction, with minima observed at an equimolar ratio for 1,2-PD with ether alcohol mixtures.

The sign and magnitude of excess functions resulting from component mixing are influenced by various factors that may act in either a synergistic or antagonistic manner. Negative contributions can arise due to several reasons, including [42]:

(a) the formation of strong molecular interactions such as ion-dipole, dipole-dipole, charge transfer (donor-acceptor) complexes, or hydrogen

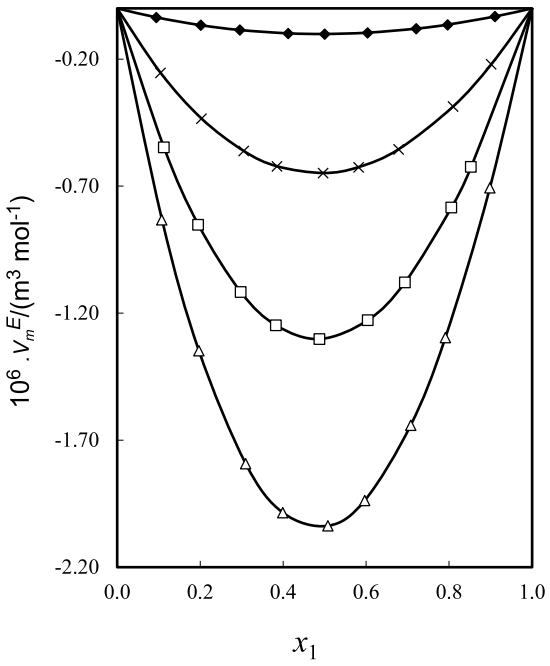

Fig. 4. Variation of excess molar volume (V_m^E) with mole fraction x_1 of 1,2-PD in the binary mixtures of 1,2-PD (1) with alkoxyalkanols (2); (◆), 2-ME; (×), 2-EE; (□), 2-PE; (Δ), 2-BE at T=298.15 K. The points represent experimental values and solid lines have been drawn from Eq. (13) using the coefficients given in Table 5.

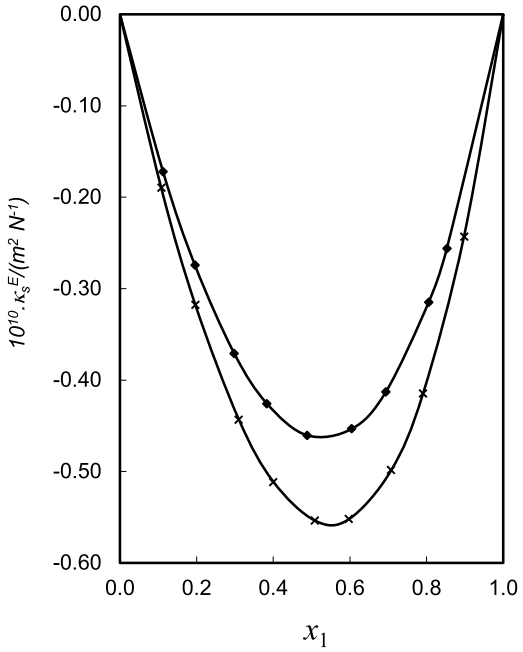

Fig. 5. Excess isentropic compressibilities (κ_s^E) with mole fraction x1 of 1,2-PD in the binary mixtures of 1,2-PD (1) with alkoxyalkanols (2); (◆), 2-PE; (×), 2-BE at T=298.15 K. The points represent experimental values and solid lines have been drawn from Eq. (13) using the coefficients given in Table 5.

bonding, among different molecules; and

(b) structural contributions stemming from the geometric fitting of molecules of one component into the interstitial spaces of molecules of the other component.

The $V_m$values of the binary systems are increasing with temperature. By observation of Figs. 1 and 2 show V_m^E are negative throughout the

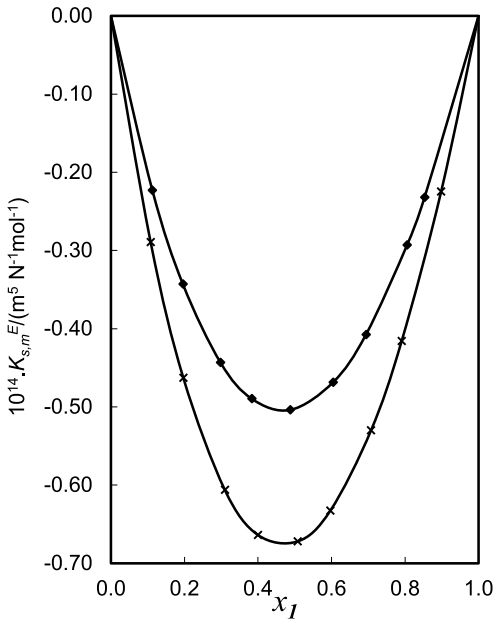

Fig. 6. Excess molar isentropic compressibilities ($K_{s,m}^E$) with mole fraction x_1 of 1,2-PD in the binary mixtures of 1,2-PD (1) with alkoxyalkanols (2); (◆), 2-PE; (×), 2-BE at T=298.15 K. The points represent experimental values and solid lines have been drawn from Eq. (13) using the coefficients given in Table 5.

mole fraction, and the values also increase as temperature increases (Table 3). From Figs. 3 and 5, the aV_m^End κ_s^Evalues for these blends are negative throughout the composition of PG at the measured temperatures.

Hydrogen Bonding: 2-PE and 2-BE are polar molecules. Each molecule has a permanent dipole moment due to the difference in electronegativity between the atoms. In Propylene glycol, the oxygen atom is more electronegative than the carbon atoms, resulting in a partial negative charge (δ^-) on the oxygen and a partial positive charge (δ^+) on the carbon atoms. Similarly, in ether alcohols, the oxygen atom in the hydroxyl group carries a partial negative charge (δ^-), while the hydrogen atom carries a partial positive charge (δ^+), which contributes to hydrogen-bond formation. When these polar molecules approach each other, the positive end of one molecule (the partially positive carbon atoms or the propyl/butyl group in ether alcohols) is attracted to the opposing end of the other molecule (the partially negative oxygen atom in propylene glycol). This alignment maximises the attractive forces between the molecules and results in dipole-dipole interactions. The negative/positive values result from the favourable or unfavourable geometric fitting of molecules of significantly different sizes into each other's structures [40].

Dipole-Dipole Interactions: Such interactions are due to the existence of polar bonds, which involve a charge separation in a molecule. Both PG and PE/BE are polar molecules, and dipole-dipole interactions can contribute to their interactions.

Structural Contribution: A careful examination of Table 3 reveals that the V_m^E values are more negative for 2-BE with PGmixture, which is caused by the larger molecules of PG leaving more voids that are occupied by smaller molecules as compared to 2-PE. The abnormal negative value of V_m^Eaffirms the existence of a powerful molecular pairing in the system.

From Fig. 4, the authors can conclude that V_m^E of PG with other 2-alkoxyalkanols follow the order: 2-BE > 2-PE > 2-EE > 2-ME at 298.15 K [64]

The V_m^Evalues also indicate that the volume contraction is most significant when considering the PG+ 2-BE system around the equimolar region. This suggests that equal molar proportions of the two compo-

nents result in the maximum non-ideality, an aspect that persists throughout the temperature domain, suggesting some interstitial accommodation that is of much larger magnitude than the other systems, as all systems share 1,2-PD as a common component.

The increase in anV_m^Ed κ_s^Evalues with rising temperatures can be attributed to structural disorder and the breaking of hydrogen bonds between different components [43]

The excess isentropic compressibility ($K_{s,m}^E$) values (Fig. 5) consistently display negativity across the range of Propylene glycol mole fractions and temperatures from 298.15 to 323.15 *K*. As the concentration of Propylene glycol increases in the binary mixtures, there is a corresponding rise in specific interactions, resulting in decreased compressibility of the mixture and hence negative excess isentropic compressibility values. This decrease in compressibility suggests enhanced rigidity within the mixture, potentially arising from local structures becoming less compressible, unlike Hydrogen bonds.

Additionally, the excess isentropic compressibility values decrease as the temperature rises (Fig.6) for these mixtures. This effect can be attributed to stronger dipole-dipole interactions that become more prominent as hydrogen bonds break with increasing temperature, resulting in more available isomeric Propylene glycol dipoles. Consequently, this closer packing of dissimilar molecules causes a volume contraction, leading to reduced molar compressibility of the mixture [43]

Throughout the complete mole fraction range, Fig.7 demonstrates that u^E values for propylene glycol (PG) with ether alcohol binary combinations are positive and go as follows: 2-PE>2-BE. By considering the orientation order of molecules in both pure liquids and the mixture, a qualitative explanation can be provided. Thermodynamically, the order within the system reflects cohesion, indicating increased intermolecular interactions. Positive u^E values suggest a heightened level of cohesion post-mixing, implying stronger intermolecular interactions compared to an ideal mixture scenario. The positive u^E values indicate notable interactions between PG and the ether alcohols in the mixture. These interactions likely involve dipole-dipole forces and hydrogen bonding between the components. Thus, the trends of u^Evs. x_1 (Fig.7) strongly supports the behaviour of V_m^E and κ_s^E for these mixtures.

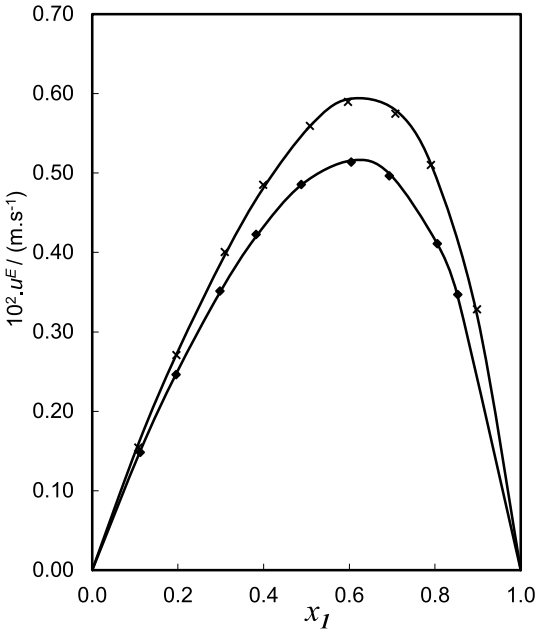

Fig. 7. Excess speed of sound (uE) with mole fraction x_1 of 1,2-PD in the binary mixtures of 1,2-PD (1) with alkoxyalkanols (2); (◆), 2-PE; (×), 2-BE at T=298.15 K. The points represent experimental values and solid lines have been drawn from Eq. (13) using the coefficients given in Table 5.

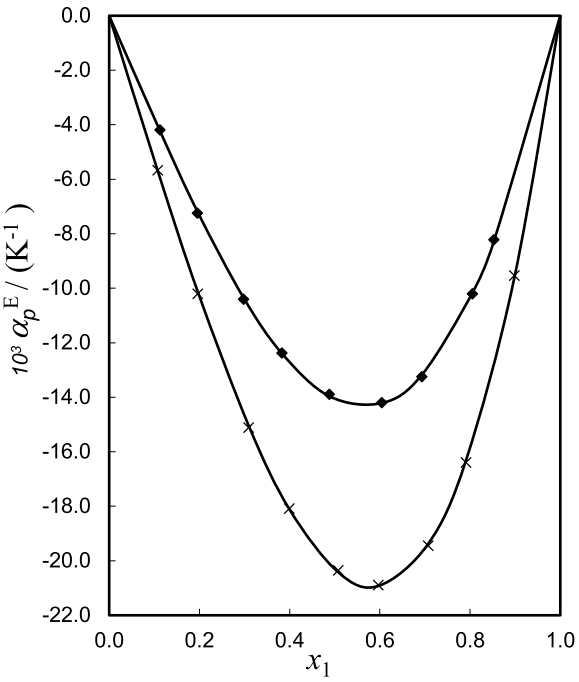

Fig. 8. Excess isobaric thermal expansivity (α_p^E) with mole fraction x_1 of 1,2-PD in the binary mixtures of 1,2-PD (1) with alkoxyalkanols (2); (◆), 2-PE; (×), 2-BE at T=298.15 K. The points represent experimental values and solid lines have been drawn from Eq. (13) using the coefficients given in Table 5.

The excess isobaric expansivity α_p^Edata of binary mixtures of PG with ether alcohol are given in Table 3, and the corresponding values are plotted against mole fraction at 298.15 *K* in Fig. 8. In order to learn more about the structural changes of the solution after mixing, the isobaric thermal expansivity at each composition is determined. Other excess volumetric properties, including excess volume and thermal compressibility, display the same general trend in these binary systems. These observations are attributed to packing effects, breaking of hydrogen bonds, and differences in the dispersion force between like and unlike

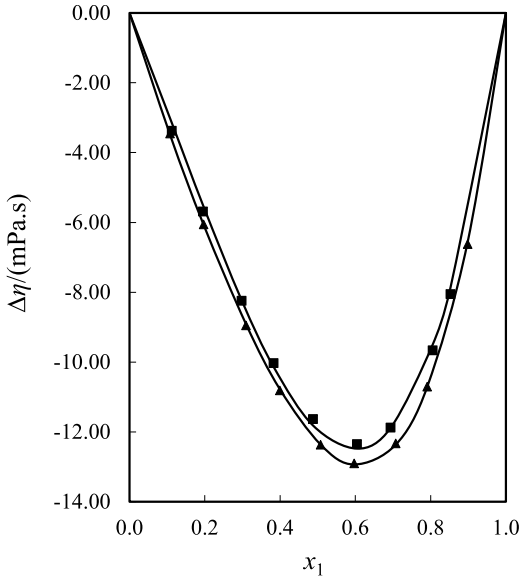

Fig. 9. Deviation in viscosity ($\Delta\eta$) with mole fraction x_1 of 1,2-PD in the binary mixtures of 1,2-PD (1) with alkoxyalkanols (2); (■), 2-PE; (▲), 2-BE; at T=298.15 K. The points represent experimental values and solid lines drawn from Eq. (13) using the coefficients given in Table 5.

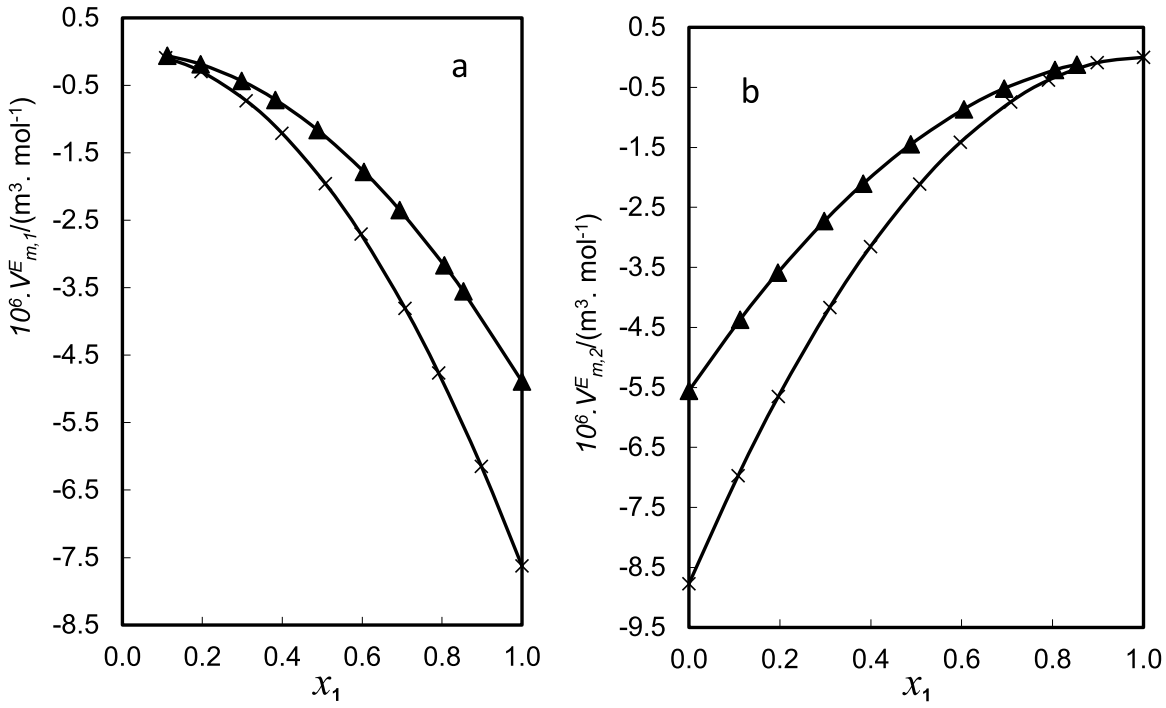

Fig. 10. Variations of excess partial molar volume ($\overline{V}^E_{m,1}$ and $\overline{V}^E_{m,2}$) with mole fraction x_1 of 1,2-PD in the binary mixtures of 1,2-PD (1) with alkoxyalkanols (2); (▲), 2-PE; (×), 2-BE at T=298.15 K.

molecules [43].

Packing effects arise from the integration of PG molecules into the hydrogen-bonded framework of the ether alcohols. This accommodation likely stems from robust interactions between unlike molecules in the mixtures [44]. Additionally, the temperature coefficient ($\partial V^E/\partial T$) is observed to be negative. This indicates the potential formation of associated species within the {PG + 2-PE/2-BE} mixture with rising temperature, leading to volume contraction and consequently negative α_p^E values.

When evaluating deviation in viscosity ($\Delta\eta$), (Table 4 & Fig.9), it is crucial to take into account the following reasons: the differences in the size and shape of the molecules involved and the breakdown of polymeric structures have a detrimental effect $\Delta\eta$ value, whereas strong and specific interactions between different compounds have a beneficial effect on $\Delta\eta$ values [45]. The negative $\Delta\eta$, across all compositions indicates a significant disruption of self-associated hydrogen bonding networks in PG, leading to a less structured liquid phase. Temperature increases weaken Hydrogen bonding, enhancing molecular ability and lowering viscosity. Additionally, steric hindrance from the bulky alkyl chain of 2-BE increases free volume, further reducing viscosity. The interplay between interaction effects (Hydrogen bonding) and non-interaction effects (molecular rearrangements) aligns with Rastogi et.al [46], where the non-interaction component dominates viscosity trends. In the present investigatory systems, the order follows PG +2-PE > PG +2-BE [47]

5. Partial molar properties

The determination of partial molar volumes and partial molar compressibility of PG, 2-PE/2-BE across the complete composition range is accomplished using Eqs. (10) and (11), in addition to other volumetric properties.

$$\overline{Y}_{m,1} = Y^E_s + Y^*_{m,1} + x_2\left(\frac{\partial Y^E_s}{\partial x_1}\right)_{T,p} \tag{10}$$

$$\overline{Y}_{m,2} = Y^E_s + Y^*_{m,2} - x_1\left(\frac{\partial Y^E_s}{\partial x_1}\right)_{T,p} \tag{11}$$

where Y is V or K_s. Where $Y^*_{m,1}$ and $Y^*_{m,2}$ are the molar components of pure molecules. The derivative $\left(\partial Y^E_s/\partial x_1\right)_{T,p}$ in Eqs. (10) and (11) are obtained by differentiation of Eq. (8), which leads to the following equations for $\overline{Y}_{m,1}$ and $\overline{Y}_{m,2}$.

$$\overline{Y}_{m,1} = \overline{Y}^*_{m,1} + x_2^2\sum_{i=0}^{j} A_i(1-2x_1)^i - 2x_1x_2^2\sum_{i=0}^{j} A_k(1-2x_1)^{i-1} \tag{12}$$

$$\overline{Y}_{m,2} = \overline{Y}^*_{m,2} + x_1^2\sum_{i=0}^{j} A_i(1-2x_1)^i + 2x_2x_1^2\sum_{i=0}^{j} A_k(1-2x_1)^{i-1} \tag{13}$$

The excess partial molar properties are calculated by the following relation [48]

$$\overline{Y}^E_{m,i} = Y^E_m + (1-x_1)\left(\partial Y^E_m/\partial x_i\right) \tag{14}$$

We aim to evaluate the partial molar properties of Propylene Glycol at infinite dilution (x_1=0) in 2-PE/2-BE, as well as the partial molar properties of 2-PE and 2-BE at infinite dilution (x_2 = 0) in Propylene Glycol. Therefore, $\overline{V}^0_{m,1}$ is obtained by setting x_1=0, which leads to

$$\overline{Y}^0_{m,1} = Y^*_{m,1} + \sum_{i=0}^{n} A_k(-1)^i \tag{15}$$

Similarly setting x_2=0, leads to

$$\overline{Y}^0_{m,2} = Y^*_{m,2} + \sum_{i=0}^{n} A_k \tag{16}$$

Here $\overline{Y}^0_{m,1}$ and $\overline{Y}^0_{m,2}$ represent the partial molar properties of Propylene Glycol at infinite dilution in ether alcohols and the partial molar properties of ether alcohols at infinite dilution in Propylene Glycol, respectively.

Table 6

The values $\overline{V}^{0}_{m,1}$, $\overline{V}^{*}_{m,1}$, $\overline{V}^{0E}_{m,1}$, $\overline{V}^{0}_{m,2}$, $\overline{V}^{*}_{m,2}$, $\overline{V}^{0E}_{m,2}$ of the components for, 1,2-PD + alkoxyethanols mixtures at temperatures T = 298.15–323.15 K from Redlich-Kister equation.

T/K	$\overline{V}^{0}_{m,1}$	$10^{6}\overline{V}^{*}_{m,1}$	$10^{6}\overline{V}^{0E}_{m,1}$	$10^{6}\overline{V}^{0}_{m,2}$	$10^{6}\overline{V}^{*}_{m,2}$	$10^{6}\overline{V}^{0E}_{m,2}$
	$10^{6}m^{3}\cdot mol^{-1}$					
1,2-PD + 2-PE						
298.15	68.130	73.685	-5.554	109.671	114.563	-4.891
303.15	68.295	73.949	-5.654	110.148	115.120	-4.972
308.15	68.465	74.220	-5.754	110.633	115.688	-5.054
313.15	68.636	74.494	-5.858	111.126	116.265	-5.139
318.15	68.807	74.772	-5.964	111.628	116.853	-5.226
323.15	68.992	75.055	-6.063	112.127	117.433	-5.305
1,2-PD + 2-BE						
298.15	64.911	73.685	-8.774	124.115	131.743	-7.628
303.15	65.025	73.949	-8.924	124.648	132.395	-7.747
308.15	65.145	74.220	-9.074	125.189	133.057	-7.868
313.15	65.268	74.494	-9.226	125.740	133.729	-7.988
318.15	65.394	74.772	-9.378	126.288	134.398	-8.110
323.15	65.524	75.055	-9.531	126.854	135.086	-8.232

Table 7

The values $\overline{\kappa}^{0}_{s,m,1}, \kappa^{*}_{s,m,1}, \overline{\kappa}^{0,E}_{s,m,1}, \overline{\kappa}^{0}_{s,m,2}, \kappa^{*}_{s,m,2}$ and $\overline{\kappa}^{0,E}_{s,m,2}$ of for the components for 1,2-PD with alkoxyalkanols at temperatures T = 298.15–323.15 K.

T/K	$\overline{\kappa}^{0}_{s,m,1}$	$\kappa^{*}_{s,m,1}$	$\overline{\kappa}^{0,E}_{s,m,1}$	$\overline{\kappa}^{0}_{s,m,2}$	$\kappa^{*}_{s,m,2}$	$\overline{\kappa}^{0,E}_{s,m,2}$
$10^{14}dm^{3}TPa^{-1}mol^{-1}$						
1,2-PD + 2-PE						
298.15	0.823	3.125	-2.303	5.649	7.446	-1.797
303.15	0.752	3.206	-2.454	5.818	7.722	-1.904
308.15	0.687	3.291	-2.604	6.009	8.012	-2.004
313.15	0.613	3.379	-2.767	6.205	8.318	-2.113
318.15	0.530	3.471	-2.941	6.409	8.639	-2.230
323.15	0.484	3.567	-3.083	6.629	8.970	-2.341
1,2-PD + 2-BE						
298.15	0.024	3.125	-3.102	6.194	8.604	-2.410
303.15	-0.075	3.206	-3.281	6.373	8.909	-2.536
308.15	-0.168	3.291	-3.459	6.573	9.228	-2.655
313.15	-0.270	3.379	-3.650	6.782	9.563	-2.782
318.15	-0.380	3.471	-3.852	6.994	9.913	-2.919
323.15	-0.453	3.567	-4.019	7.232	10.281	-3.049

Excess partial molar properties at infinite dilution $\overline{Y}^{0,E}_{m,i}$ for each component in binary liquid, mixtures is evaluated through relations

$$\overline{Y}^{0,E}_{m,1} = \overline{Y}^{0}_{m,1} - Y^{*}_{m,1} \tag{22}$$

$$\overline{Y}^{0,E}_{m,2} = \overline{Y}^{0}_{m,2} - Y^{*}_{m,2} \tag{23}$$

The partial molar volumes in the studied systems are indicative of the molecular interactions present. These partial molar volumes result from various factors including the intrinsic volume of the dipolar molecules, the electrostriction caused by the solvent, and contributions from the molecular structure. The partial molar volumes $\overline{V}_{m,1}$ and $\overline{V}_{m,2}$ and excess partial molar volumes $\overline{V}^{E}_{m,1}$ and $\overline{V}^{E}_{m,2}$ as a function of the mole fractions of PG and temperature are provided in Table 5S. The variations $\overline{V}^{E}_{m,1}$ and $\overline{V}^{E}_{m,2}$ with compositions at 298.15 K as shown in Fig. 10. The values of $\overline{V}^{0}_{m,1}, \overline{V}^{*}_{m,1}, \overline{V}^{0,E}_{m,1}, \overline{V}^{0}_{m,2}, \overline{V}^{*}_{m,2}$ and $\overline{V}^{0,E}_{m,2}$ for both the blended mixtures at the measured temperatures, the values are listed in Table 6.

It was found that the excess molar volumes of both components, $\overline{V}^{E}_{m,1}$ and $\overline{V}^{E}_{m,2}$ are negative throughout the entire composition range. This suggests that the molar volumes of the components in the mixture are smaller than their individual molar volumes in the pure state, indicating a volume contraction when PG is mixed with ether alcohols. This contraction is due to the disruption of self-association in 2-PE/2-BE molecules and the formation of Hydrogen bonds between different molecules. Additionally, the excess partial molar volumes increase with temperature, implying that higher temperatures weaken the donor-acceptor interactions between the molecules, resulting in volume expansion.

It was found that the excess molar volumes of both components, $\overline{V}^{E}_{m,1}$ and $\overline{V}^{E}_{m,2}$ are negative throughout the entire composition range. This suggests that the molar volumes of the components in the mixture are smaller than their individual molar volumes in the pure state, indicating a volume contraction when PG is mixed with ether alcohols. This contraction is due to the disruption of self-association in 2-PE/2-BE molecules and the formation of hydrogen bonds between different molecules. Additionally, the excess partial molar volumes increase with temperature, implying that higher temperatures weaken the donor-acceptor interactions between the molecules, resulting in volume expansion.

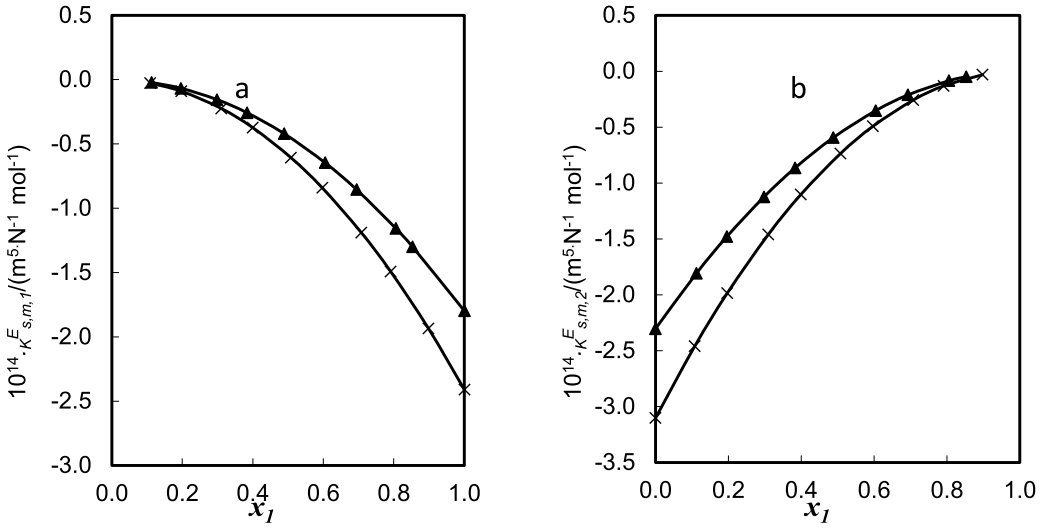

Fig. 11. Excess partial molar compressibilities ($\overline{K}^{E}_{s,m,1}$ and $\overline{K}^{E}_{s,m,2}$) with mole fraction x_1 of 1,2-PD in the binary mixtures of 1,2-PD (1) with alkoxyalkanols (2); (▲), 2-PE; (×), 2-BE at T=298.15 K.

$\overline{K}_{s,m,1}$,$\overline{K}_{s,m,2}$ and $\overline{K}^{E}_{s,m,1}$, $\overline{K}^{E}_{s,m,2}$ values were presented at T = 298.15 - 323.15 K in Table 6S. In Table 7, $\overline{K}^{0}_{s,m,1}$,$\overline{K}^{*}_{s,m,1}$,$\overline{K}^{0,E}_{s,m,1}$, $\overline{K}^{0}_{s,m,2}$, $\overline{K}^{0,*}_{s,m,2}$ and $\overline{K}^{0,E}_{s,m,2}$ values were presented for the investigated temperatures. From Fig.11 $\overline{K}^{E}_{s,m,1}$ and $\overline{K}^{E}_{s,m,2}$ were negative and increased with temperature. This indicates that when PG was mixed with 2-PE/2-BE, the molar isentropic compressibility of both components decreased, compared to their molar isentropic compressibilities in their pure forms. In general, the negative $\overline{K}^{E}_{s,m,1}$ and $\overline{K}^{E}_{s,m,2}$ values indicate stronger (solute + solvent) interactions than similar molecule interactions, whereas the positive $\overline{K}^{E}_{s,m,1}$ and $\overline{K}^{E}_{s,m,2}$ values indicate weak interactions between similar components [49] in the blends. The magnitude of $\overline{K}^{E}_{s,m,1}$ and $\overline{K}^{E}_{s,m,2}$ at mole fraction ≈0.5 follows the sequence: 2-PE < 2-BE. This is caused by the Hydrogen bonding strength of ether alcohols increasing with chain length [50]. In terms of Hall [51] and others [52] the $\overline{K}^{E}_{s,m,1}$ & $\overline{K}^{E}_{s,m,2}$ values were negative due to structural and geometrical compressibility. Structural compressibility arises from the disruption of the associated structure, while geometrical compressibility results from the concurrent compression of the molecules. This is due to specific interactions between PG and 2-PE/2-BE, which lead to a reduction in volume and a decrease in average intermolecular distances. Also, the $\overline{K}^{E}_{s,m,1}$ and $\overline{K}^{E}_{s,m,2}$ values increase concerning temperature (Table 5S) for each binary mixture under this study.

5. Modelling

5.1. Liquid density using PC-SAFT EOS

This theoretical model states that the liquid density can be obtained with Eq. (23)

$$\left[\rho\left(\frac{\partial a}{\partial \rho}\right)_{T,V} - a\right] = P \tag{23a}$$

Where a= A/V is the Helmholtz energy density, A represents the molar Helmholtz energy, V is the molar volume, T denotes the temperature, ρ is the molar density, and P is the absolute pressure at 0.1 MPa.

From PC-SAFT EoS, the Helmholtz energy is given by Eq. (24)

$$A = A^{ig} + A^{disp} + A^{assoc} \tag{24}$$

Where A^{ig}, A^{disp} and A^{assoc} are related to the ideal gas term, a hard-chain contribution, London forces, and association term respectively. Each of the above contributions has been widely discussed in the literature [25,26]

In this equation of state, each pure component requires five fitted parameters: the segment diameter that does not vary with temperature (σ), the number of segments (m), the energy parameter (ε), the effective volume (κ^{AB}), and the association energy parameter (ε^{AB}). When there is no association in the pure fluids, the last two parameters are assigned a value of zero. On the other hand, for the application of PC-SAFT to mixtures it is necessary to analyze the parameter k_{ij}. This is a parameter adjusted to account for interactions caused by London dispersion forces. To use a fully predictive model for obtaining the density in multicomponent mixtures, we have chosen to set k_{ij} to exactly zero.

5.2. Speed of sound using SCFT and NR

One key benefit of these models SCFT [27] and NR [28] is that don't require fitted parameters to the experimental viscosity data for binary mixtures. The speed of sound (u) defined as SCFT is given by Eq.25

$$u = 1600\rho\left(\sum_{i=1}^{n_c} x_i s_i\right)\left(\sum_{i=1}^{n_c} x_i N_{av} m_i \frac{\pi}{6} d_i^3\right) \tag{25}$$

Where n_c denotes the number of components in the mixture x_i denotes the liquid mole fraction, N_{av} represents the Avogadro constant, and d_i is the segment diameter dependent on temperature defined as PC-SAFT EoS [25,26] and s_i indicates the space-filling factor of fluid in the mixture.

Moreover, from NR model [28] the speed if sound is defined as Eq. (26)

$$u = \left(\frac{\sum_{i=1}^{n_c} \frac{x_i}{\rho_i} u_i^{1/3}}{\sum_{i=1}^{n_c} \frac{x_i}{\rho_i}}\right)^3 \tag{26}$$

Where u_i and ρ_i, the experimental speed of sound and molar density of pure liquid respectively.

5.3. Viscosity using FVT

Allan et al [29–31] propose that dynamic viscosity from FVT is defined as Eq. (27)

$$\eta = \eta^0 + \Delta\eta \tag{27}$$

Where η^0 and Δη represents the viscosity of dilute gas and the residual viscosity, respectively. The expression for the viscosity of dilute gas is given by Chung et al, [53], while that residual gas is expressed as Eq. (28)

$$\Delta\eta = 1000\widehat{\rho} l \left(\frac{\alpha + \frac{MP}{\widehat{\rho}}}{\sqrt{3MRT}}\right) \exp\left[B\left(\frac{\alpha + \frac{MP}{\widehat{\rho}}}{2RT}\right)^{1.5}\right] \tag{28}$$

Where Δη is the residual viscosity in mPa.s, R represents the universal gas constant in J•mmo^{l-1}•K^{-1}, M denotes the molar mass in kg•mol^{-1}, P is the absolute pressure in Pa, $\widehat{\rho}$is the liquid density in kg.m^{-3}, which is obtained from PC-SAFT EoS.

FVT has three fitted parameters for the pure fluids, which are fitted with experimental viscosity data. These parameters are α, B, and l, which represent the barrier energy, free volume overlap and characteristic molecular length. To obtain the residual viscosity in mPa.s, it's necessary that the previously fitted parameters be in the following units: J.mol^{-1}, dimensionless and m, respectively.

The calculation of viscosity in mixtures requires the use of mixing rules η^0 and Δη. The viscosity of dilute gas for the mixture can be obtained from Eq. 29.

$$\eta_0 = \exp\left[\sum_{i=1}^{n_c} x_i \ln\left(\eta_{0,i}\right)\right] \tag{29}$$

Where, $\eta_{0,i}$denotes the viscosity of dilute gas for the pure liquid i. On the other hand, the calculation of the residual viscosity of the mixture is obtained with Eq. (28) but coupled to the mixing rules defined by Eq. (30), (31) & (32).

$$\alpha_m = \sum_{i=1}^{n_c}\sum_{j=1}^{n_c} x_i x_j \sqrt{\alpha_i \alpha_j}\left(1 - l_{ij}\right) \tag{30}$$

$$B_m = \sum_{i=1}^{n_c}\sum_{j=1}^{n_c} x_i x_j \sqrt{B_i B_j}\left(1 - w_{ij}\right) \tag{31}$$

$$l_m = \sum_{i=1}^{n_c}\sum_{j=1}^{n_c} x_i x_j \sqrt{l_i l_j}\left(1 - u_{ij}\right) \tag{32}$$

Where the mixture parameters (α_m, B_m, l_m) are assumed to exhibit a quadratic dependence on the mole fraction. According to the above equations, we observe three fitted parameters (l_{ij}, wi_j, ui_j) which are obtained by fitting experimental viscosity data of mixtures.

Table 8
Parameters for the pure fluids required in PC-SAFT EoS and the absolute average deviation for the vapor pressure and liquid density. The temperature range was 298.15 K to 323.15 K.

Fluid	m	σ / (Å)	ε/k_B / (K)	κ^{AB}	ε^{AB}/k_B / (K)	%*AADP*	%*AAD*ρ
1,2-Propanediol	2.09998	3.77878	379.07019	0.0071067	1821.47	0.08	0.01
2-Propoxyethanol	2.49998	4.04146	324.04260	0.0019462	2016.43	0.03	0.01
2-Butoxyethanol	2.89998	4.02831	308.31348	0.010504	1620.50	0.04	0.06
Overall						0.05	0.03

Table 9
The average deviation for liquid density of the binary mixtures considering all the temperatures (298.15 K, 303.15 K, 313.15 K, 318.15 K, and 323.15 K). The calculations were obtained using PC-SAFT EoS.

Mixture	%*AAD*ρ
1,2-Propanediol (1) + 2-Propoxyethanol (2)	0.42
1,2-Propanediol (1) + 2-Butoxyethanol (2)	0.87
Overall	0.65

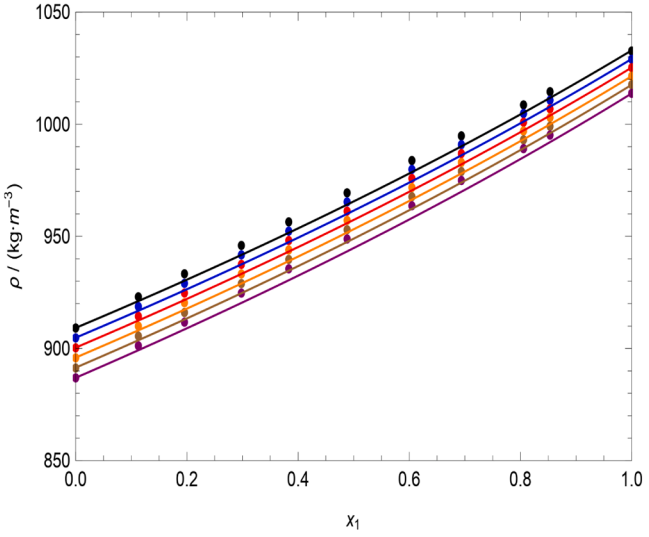

Fig. 12. Comparison between experimental density and calculated density using PC-SAFT EoS for the 1,2-propanediol (1) + 2-propoxyethanol (2) mixture at different temperatures and 0.1 MPa. Circles denote the experimental data at temperatures : (black) 298.15 K, (blue) 303.15 K, (red) 308.15 K, (orange) 313.15 K, (brown) 318.15 K, (purple) 323.15 K. Lines represent the theoretical data obtained with PC-SAFT and $k_{ij} = 0$.

Before optimising the fitted parameters of PC-SAFT EoS, it is required to select the association scheme for each pure fluid. For PG, a 4C scheme was assumed, i.e, 2 positive sites on the hydrogen atoms of OH groups, and two negative sites on the oxygen atoms, while in 2-propoxyethanol and 2-butoxyethanol, due to the presence of the OH group and oxygen atom, a 3B scheme was assumed (2 negative sites, one on each oxygen atom, and 1 positive site on the hydrogen atom of OH group). Therefore, the parameters (m, σ, $\frac{\varepsilon}{k_B}$, $\frac{\varepsilon^{AB}}{k_B}$, κ^{AB}) were optimized using vapor pressure data from DIPPR [54] and experimental compressed liquid density data (published in this work). In this manuscript, we have used the objective function expressed by Eq. 33

$$OF\left(m,\sigma,\frac{\varepsilon}{k_B},\frac{\varepsilon^{AB}}{k_B},k^{AB}\right) = \min\sum_{i=1}^{n}\left(\frac{P_i^{calc}-P_i^{DIPPR}}{P_i^{DIPPR}}\right)^2 + \left(\frac{\rho_i^{calc}-\rho_i^{\exp}}{\rho_i^{\exp}}\right)^2 \quad (33)$$

where, calc. and exp. are related to the calculated value with the theoretical model and experimental value, respectively. N indicates the number of experimental data. On the other hand, the absolute average deviation was obtained from Eq. (34).

$$AAD\psi(\%) = \frac{100}{N}\sum_{i=1}^{N}\frac{\left|\psi_i^{\exp}-\psi_i^{th}\right|}{\psi_i^{\exp}} \quad (34)$$

where, Ψ is the property (density, speed of sound, and viscosity).

Then, the optimal parameters in the temperature range of 298.15 K to 323.15 K and the deviations obtained are summarised in Table 8.

According to the results obtained in Table 8, it is observed that the number of spherical segments is greater in the following order: 2-butoxyethanol > 2-propoxyethanol > 1,2-propanediol. Furthermore, the % AAD obtained in both vapour pressure and liquid density is meagre, which implies an excellent agreement of our model with the experimental data. For density modelling in binary mixtures, we have used a fully predictive approach for mixtures ($k_{ij} = 0$), and the deviations obtained are published in Table 9.

Table 9, shows good quantitative agreement between theoretical and experimental data for both mixtures over the temperature range of 298.15 -323.15 K and mole fraction range of 0 to 1. On the other hand, the overall deviation in liquid density is 0.65%.

Furthermore, the variation of liquid density with the mole fraction of 1,2-propanediol for different temperatures is observed in Fig 11 and 12

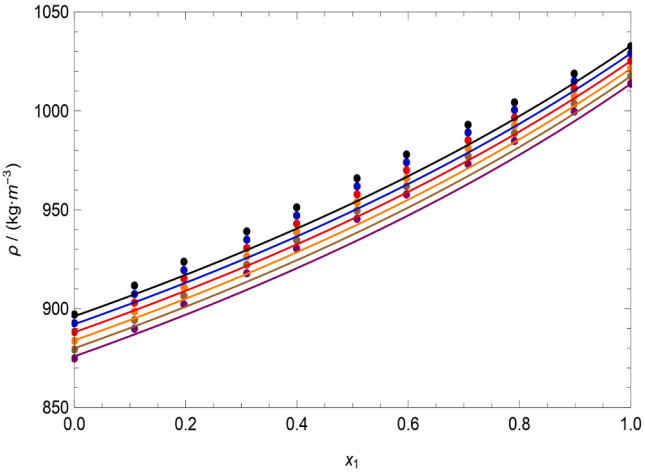

Fig. 13. Comparison between experimental density and calculated density using PC-SAFT EoS for the 1,2-propanediol (1) + 2-butoxyethanol (2) mixture at different temperatures and 0.1 MPa. Circles denote the experimental data at temperatures: (black) 298.15 K, (blue) 303.15 K, (red) 308.15 K, (orange) 313.15 K, (brown) 318.15 K, (purple) 323.15 K. Lines represent the theoretical data obtained with PC-SAFT and $k_{ij} = 0$.

Table 10
The average deviation for speed of sound of the binary mixtures considering all the temperatures (298.15 K, 303.15 K, 313.15 K, 318.15 K, and 323.15 K). The calculations were obtained using SCFT + PC-SAFT EoS and NR + PC-SAFT EoS.

Mixture	SCFT	NR
1,2-Propanediol (1) + 2-Propoxyethanol (2)	0.09	1.47
1,2-Propanediol (1) + 2-Butoxyethanol (2)	0.30	1.77
Overall	0.20	1.62

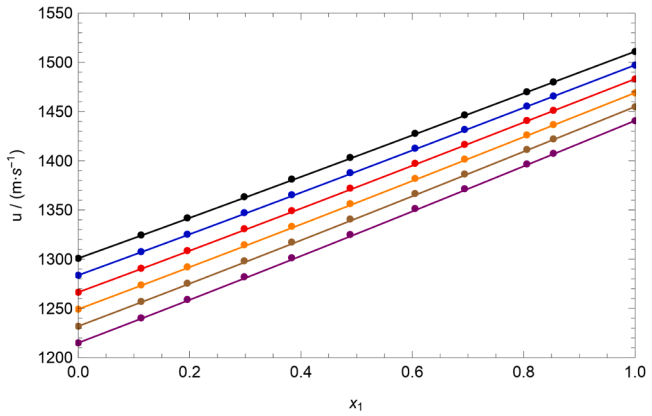

Fig. 14. Comparison between experimental speed of sound and calculated speed of sound using SCFT + PC-SAFT EoS for the 1,2-propanediol (1) + 2-propoxyethanol (2) mixture at different temperatures and 0.1 MPa. Circles denote the experimental data at temperatures: (black) 298.15 K, (blue) 303.15 K, (red) 308.15 K, (orange) 313.15 K, (brown) 318.15 K, (purple) 323.15 K. Lines represent the theoretical data obtained with SCFT + PC-SAFT and $k_{ij} = 0$.

for the 1,2-propanediol + 2-propoxyethanol and 1,2-propanediol + 2-butoxyethanol mixtures, respectively.

Then, from Figs. 12 and 13 we can see that there is good qualitative and quantitative agreement, that the influence of dispersive forces and hydrogen bonding forces on density computation are well modelled with PC-SAFT EoS. Furthermore, according to our results (theoretical and experimental), an approximately linear behaviour of the density with the mole fraction of 1,2-propanediol is obtained.

The results related to modelling the speed of sound using SCFT and NR will be described below. First of all, it is necessary to comment that with these models we cannot calculate the speed of sound in pure fluids, however, it can be applied to mixtures, but it is necessary to take as input the experimental value of the speed of sound in pure fluids. Therefore, the deviations obtained are shown in Table 10.

From Table 10, both models can correctly model the experimental speed of sound from a quantitative point of view; however, the best results were obtained with SCFT. The visualization of these results graphically obtained with SCFT will be illustrated in Figs. 14 and 15 for the mixtures of 1,2-propanediol with 2-propoxyethanol and 2-butoxyethanol, respectively.

The observed higher deviation in speed of sound predictions using Nomoto's Relation (NR), compared to Schaaff's Collision Factor Theory (SCFT), arises from their inherent modeling assumptions. NR is an empirical rule based on ideal additive volume and density relations, and it assumes no significant molecular interactions between components. As such, it tends to fail in systems where strong hydrogen bonding or specific dipolar interactions are present, such as in PG - ether alcohol mixtures. In contrast, SCFT incorporates molecular packing and space-filling parameters derived from PC-SAFT density inputs, making it more physically grounded and sensitive to molecular association effects. Hence, SCFT better captures the influence of hydrogen bonding and structural compactness in these mixtures, resulting in lower prediction error. This suggests that while NR may be suitable for weakly interacting systems, SCFT provides superior accuracy for strongly interacting or non-ideal liquid mixtures.

According to the previous figures, SCFT + PC-SAFT correctly models the linear dependence of the speed of sound on the mole fraction of 1,2-propanediol. It's important to note again that the theoretical results for the speed of sound are purely predictive for mixtures.

For Viscosity modelling in pure fluids at 0.1Mpa and at temperatures of 298.15 and 303.15 K, we utilize the DPRR database along with saturated liquid viscosity data. The objective function is defined as shown in Eq. (35).

$$OF(\alpha, B, l) = \min \sum_{i=1}^{N} \left(\frac{\eta_i^{calc} - \eta_i^{DIPPR}}{\eta_i^{DIPPR}} \right)^2 \quad (35)$$

According to the results of Table 11, we observe that the three fitted parameters to the DIPPR data show good agreement (overall deviation is 0.31%) between our model and those used. For the case of binary mixtures, we used the FVT model as a fitted approach, where the parameters (l_{ij}, w_{ij}, and u_{ij}) were optimized using our experimental compressed liquid viscosity data and the objective function given by Eq.36

Table 11
Fitted parameters for the pure fluids required in FVT and the absolute average deviation for the viscosity. The temperature range was 298.15 K to 323.15 K.

Fluid	α / (Jmol^{-1})	B	l / (Å)	%$AAD\eta$
1,2-Propanediol	76817.71	0.17646	0.0026126	0.76
2-Propoxyethanol	52616.31	0.14980	0.087243	0.08
2-Butoxyethanol	42119.51	0.21747	0.10402	0.09
Overall				0.31

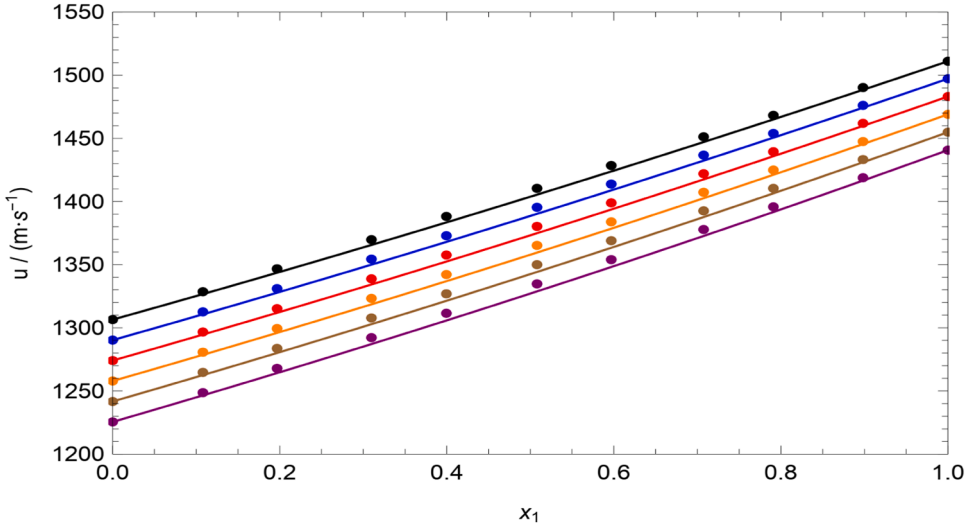

Fig. 15. Comparison between experimental speed of sound and calculated speed of sound using SCFT + PC-SAFT EoS for the 1,2-propanediol (1) + 2-butoxyethanol (2) mixture at different temperatures and 0.1 MPa. Circles denote the experimental data at temperatures : (black) 298.15 K, (blue) 303.15 K, (red) 308.15 K, (orange) 313.15 K, (brown) 318.15 K, (purple) 323.15 K. Lines represent the theoretical data obtained with SCFT + PC-SAFT and $k_{ij} = 0$.

Table 12
Fitted parameters for the binary mixtures required in FVT and the absolute average deviation for the viscosity.

Mixture	T / (K)	l_{ij}	w_{ij}	u_{ij}	%$AAD\eta$
1,2-Propanediol (1) + 2-Propoxyethanol (2)	298.15 K, 303.15 K	-0.13035	0.23229	0.32733	1.46
1,2-Propanediol (1) + 2-Butoxyethanol (2)	298.15 K	0.00048902	0.12853	0.30296	2.38
	303.15 K	0.16631	-0.14192	0.43767	
Overall					1.92

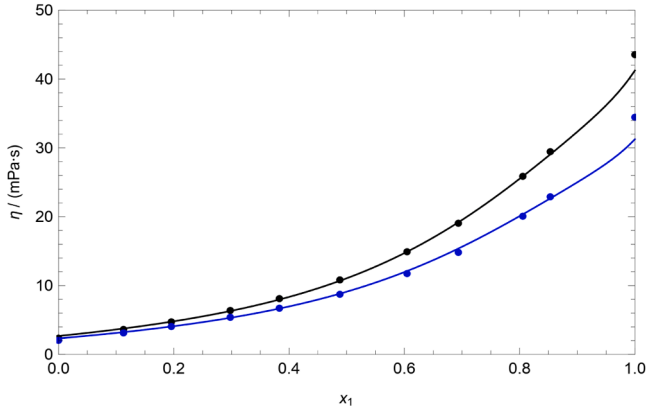

Fig. 16. Comparison between experimental viscosity and calculated viscosity using FVT + PC-SAFT EoS for the 1,2-propanediol (1) + 2-propoxyethanol (2) mixture at different temperatures and 0.1 MPa. Circles denote the experimental data at temperatures: (black) 298.15 K, (blue) 303.15 K. Lines represent the theoretical data obtained with FVT + PC-SAFT, $k_{ij} = 0$, $l_{ij} = -0.13035$, $w_{ij} = 0.23229$, and $u_{ij} = 0.32733$.

$$OF(\alpha, B, l) = \min \sum_{i=1}^{N} \left(\frac{\eta_i^{calc} - \eta_i^{Exp}}{\eta_i^{Exp}} \right)^2 \quad (36)$$

The optimized parameters and the obtained deviations are available in Table 12. For the 1,2-propanediol + 2-propoxyethanol mixture, the parameters were optimized using both temperatures in the adjustment, while for the other mixture, the parameters were optimized for each temperature; this approach was used to improve our results (obtain less

Table 13
The values of reduced volume,$\widetilde{V}$, characteristic volume, V*, characteristic pressure, P*, characteristic temperature, T*, isothermal compressibility, κ_T, isentropic compressibility, κ_s,and thermal expansion coefficient, α of pure liquids at temperatures, T = (298.15 to 323.15) K.

T/K	$\widetilde{V}$	V* 10^6 $m^3.mol^{-1}$	P* 10^{-8} $J.cm^{-3}$	T*/K	κ_T 10^{10} $m^2.N^{-1}$	κ_s 10^{10} $m^2.N^{-1}$	α 10^4 K^{-1}
1,2-PD							
298.15	1.1867	62.09	6.225	6380	4.836	4.242	12.479
303.15	1.1898	62.15	6.249	6407	4.938	4.336	12.558
305.15	1.1956	62.08	6.367	6374	5.064	4.434	12.637
313.15	1.2011	62.02	6.474	6348	5.192	4.537	12.718
318.15	1.2046	62.07	6.488	6371	5.315	4.642	12.799
323.15	1.2104	62.01	6.591	6343	5.459	4.752	12.881
2-PE							
298.15	1.1595	76.741	5.568	7183	4.318	3.848	5.998
303.15	1.1623	76.786	5.610	7206	4.392	3.916	6.016
305.15	1.1651	76.831	5.650	7229	4.467	3.986	6.034
313.15	1.1679	76.878	5.688	7253	4.544	4.058	6.052
318.15	1.1708	76.924	5.726	7276	4.623	4.131	6.070
323.15	1.1736	76.973	5.761	7299	4.704	4.207	6.089
2-BE							
298.15	1.2456	105.768	5.765	5261	7.940	6.531	7.652
303.15	1.2500	105.916	5.766	5286	8.170	6.729	7.681
305.15	1.2544	106.069	5.764	5311	8.409	6.936	7.711
313.15	1.2589	106.227	5.758	5336	8.658	7.151	7.741
318.15	1.2633	106.382	5.748	5362	8.919	7.376	7.771
323.15	1.2678	106.549	5.739	5387	9.185	7.611	7.801

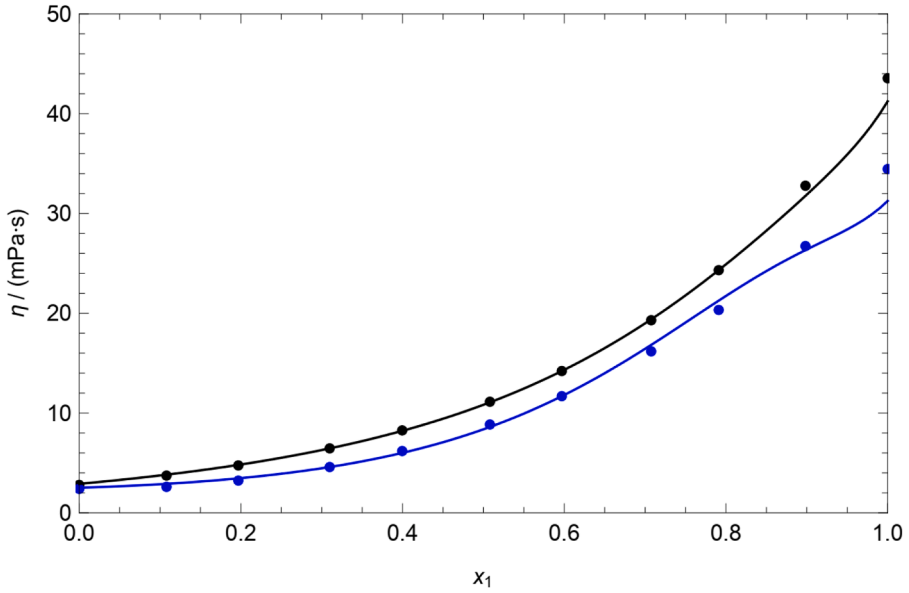

Fig. 17. Comparison between experimental viscosity and calculated viscosity using FVT + PC-SAFT EoS for the 1,2-propanediol (1) + 2-butoxyethanol (2) mixture at different temperatures and 0.1 MPa. Circles denote the experimental data at temperatures: (black) 298.15 K, (blue) 303.15 K. Lines represent the theoretical data obtained with FVT + PC-SAFT at 298.15 K: $k_{ij} = 0$, $l_{ij} = 0.00048902$, $w_{ij} = 0.12853$, and $u_{ij} = 0.30296$, and at 303.15 K: $k_{ij} = 0$, $l_{ij} = -0.16631$, $w_{ij} = -0.14192$, and $u_{ij} = 0.43767$.

Table 14
Values of χ_{12}, θ_2, experimental and calculated V_m^E (using PFP theory) and three PFP contributions for near equimolar composition at temperatures, T = (298.15 to 323.15) K.

T/K	θ_2	χ_{12} 10^{-8} $J.mol^{-1}$	V_m^E 10^6 $m^3.mol^{-1}$				
			Expt	PFP	PFP contribution to V_m^E		
					int.	fv	ip
1,2-PD + PE							
298.15	0.5772	-1.181	-1.4144	-1.4106	-1.115	-0.088	-0.088
303.15	0.5773	-1.163	-1.4551	-1.4504	-1.125	-0.092	-0.096
308.15	0.5777	-1.145	-1.4995	-1.4954	-1.133	-0.088	-0.115
313.15	0.5781	-1.128	-1.5474	-1.5433	-1.142	-0.084	-0.133
318.15	0.5782	-1.111	-1.5880	-1.5831	-1.155	-0.087	-0.141
323.15	0.5786	-1.095	-1.6376	-1.6327	-1.165	-0.083	-0.157
1,2-PD + BE							
298.15	0.5801	-1.857	-1.4144	-1.4106	-1.859	-0.104	-0.090
303.15	0.5802	-1.835	-1.4551	-1.4504	-1.881	-0.109	-0.096
308.15	0.5806	-1.812	-1.4995	-1.4954	-1.898	-0.105	-0.117
313.15	0.5810	-1.791	-1.5474	-1.5433	-1.918	-0.101	-0.135
318.15	0.5811	-1.766	-1.5880	-1.5831	-1.940	-0.105	-0.142
323.15	0.5815	-1.746	-1.6376	-1.6327	-1.962	-0.100	-0.159

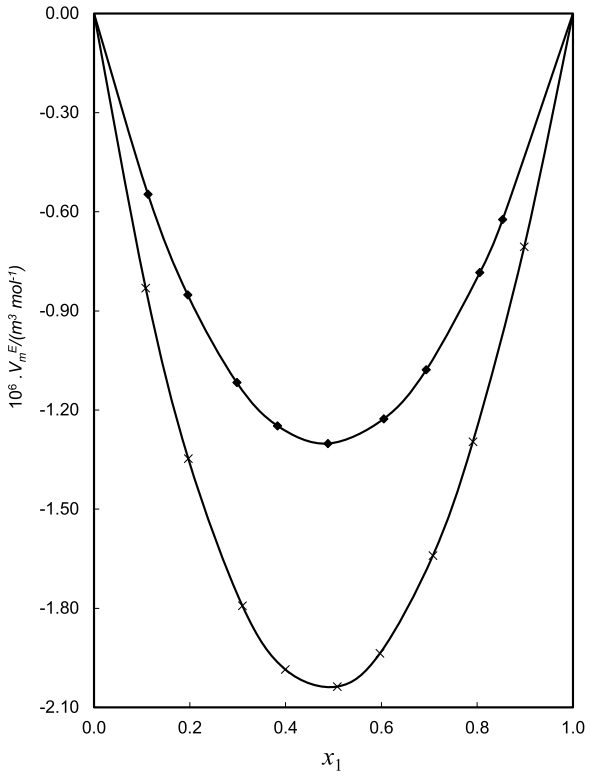

Fig. 18. Plot of excess molar volumes vs. mole fraction of 1.2-PD in the binary mixtures of 1,2-PD (1) with alkoxyalkanols (2); (◆), 2-PE; (x), 2-BE; Experimental (points) and solid lines have been drawn from PFP theory.

deviation in the modelling). On the other hand, with our optimal parameters, we observe good quantitative agreement and an overall deviation of 1.92%.

Finally, Figs. 16 and 17 show the behaviour of viscosity with the mole fraction of 1,2-propanediol for the mixtures with 2-propoxyethanol and 2-butoxyethanol, respectively. According to these figures, FVT coupled to the fitted parameters correctly represents the experimental data. Furthermore, they correctly model the dependence of viscosity on mole fraction and temperature.

6. Prigogine–Flory–Paterson (PFP) model

Three main contributions are made to excess molar volume estimations by the Prigogine–Flory–Paterson (PFP) Model: (i) The interaction parameters (χ_{12}) determine the proportionality of this component. (ii) Free Volume Contribution: This results from the lowered volume depending on the reduced temperature, which reflects the variations in the expansion rates of the two components. (iii) P* Contribution: The variations in the component decreased volumes, as well as the variations in internal pressures, determine this.

The excess molar volume is computed using the Prigogine–-Flory–Paterson theory, which incorporates these three contributions in the following equation.

$$\frac{V^E}{x_1V_1^* + x_2V_2^*} = \frac{\left(\tilde{V}^{1/3}-1\right)\tilde{V}^{2/3}}{\left[(4/3)\tilde{V}^{-1/3}-1\right]}\Psi_1\theta_2\left(\frac{\chi_{12}}{P_1^*}\right) - \frac{(V_1-V_2)^2\left[(14/9)\tilde{V}^{-1/3}-1\right]\Psi_1\Psi_2}{\left[(4/3)\tilde{V}^{-1/3}-1\right)\tilde{V}} + \frac{(\tilde{V}_1-\tilde{V}_2)(P_1^*-P_2^*)}{P_1^*\Psi_2+P_2^*\Psi_1}\Psi_1\Psi_2 \quad (33a)$$

In Eq. (23) the first term relates to the interactional contribution V_m^E(int), the second term is the free volume contribution V_m^E(fv), and the last term relates to the internal pressure contribution V_m^E(P*). The values of pure parameters for the pure liquid components and the mixture are obtained by Flory theory (Table 13).

From Table 14, χ_{12}values were observed as negative for the investigated mixtures, thereby suggesting a significant intermolecular interaction between the molecules of the mixtures, which is also supported by the negative V_m^E values of the mixture. The interaction parameters of contribution internal pressure V_m^E (int.), internal pressure V_m^E (ip), and free volumeV_m^E (fv.) were negative for both cases of 2-PE & 2-BE. In these parameters, the major contribution is that the interaction parameter values were larger compared to the other two parameters, and in the case of 2-BE, these values are high compared with 2-PE. Fig. 18 illustrates how well the Prigogine-Flory-Paterson (PFP) theory predicts V_m^Evalues for the systems under study at 298.15 K and throughout the whole PG range. This demonstrates unequivocally that 2-PE > 2-BE is the order in which these systems interact. This is a good agreement with the conclusions drawn from V_m^E, κ_s^E, u^E, $K_{s,m}^E$, α_p^E, $\Delta\eta$ $\overline{V}_{m,1}^E$ and $\overline{V}_{m,2}^E$, and $\overline{K}_{s,m,1}^E$ and $\overline{K}_{s,m,2}^E$ values of these binary blends.

Table 15
Values of parameters calculated from various one-, two-, and three-parameter models of viscosity, along with the average percentage deviations, σ (%) between theoretical and experimental η values for the binary mixture at T/K = 298.15 and 303.15.

T/K	Model	Parameter			APD (%)
	2-PE+1,2-PD				
298.15	Grunberg-Nissan	G_{12} =0.34			2.91
	Hind *et al*	H_{12} = -0.97			17.18
	Katti-Chaudhri	W_{vis}/RT = 0.40			2.85
	Heric-Brewer (2-parameter)	α_{12} = 0.48	A_{21} = -0.23		1.41
	McAllister (3-body int)	Z_{12} = 22.32	Z_{21} = 12.36		12.99
	Lobe	α_{12} = 0.48	α_{21} = -0.89		0.61
	Heric-Brewer (3-parameter)	a = 1.11	b = -1.25	c = 1.04	16.06
	McAllister (4-body int)	Z_{1112} =22.63	Z_{1122} = 11.19	Z_{1222} = 5.13	4.04
	Auslander	A_{21} = 1.66	B_{12} = 7.04	B_{21} = 0.38	0.30
303.15	Grunberg-Nissan	G_{12} = 0.15			2.58
	Hind *et al*	H_{12} = 0.79			15.18
	Katti-Chaudhri	W_{vis}/ RT=0.21			3.58
	Heric-Brewer (2-parameter)	α_{12} = 0.36	A_{21} = -0.44		1.25
	McAllister (3-body int)	Z_{12} = 16.33	Z_{21} = 10.74		13.94
	Lobe	α_{12} = 0.37	α_{21} = -0.37		0.85
	Heric-Brewer (3-parameter)	a = 0.98	b = -1.506	c = 1.17	18.67
	McAllister (4-body int)	Z_{1112} = 17.44	Z_{1122} = 7.98	Z_{1222} = 5.26	1.63
	Auslander	A_{21} = 7.57	B_{12} = 28.75	B_{21} = 0.08	0.78
	2-BE+1,2-PD				
298.15	Grunberg-Nissan	G_{12} =-0.03			10.38
	Hind *et al*	H_{12} = -1.34			9.23
	Katti-Chaudhri	W_{vis}/RT = 0.04			10.15
	Heric-Brewer (2-parameter)	α_{12} = 0.22	A_{21} = 0.78		4.34
	McAllister (3-body int)	Z_{12} = 24.40	Z_{21} = 11.10		37.79
	Lobe	α_{12} = 0.53	α_{21} = -1.00		10.87
	Heric-Brewer (3-parameter)	a = 0.972	b = -1.188	c = 0.922	33.71
	McAllister (4-body int)	Z_{1112} =21.83	Z_{1122} = 10.92	Z_{1222} = 5.5	24.11
	Auslander	A_{21} = 0.72	B_{12} = 3.95	B_{21} = 0.75	9.27
303.15	Grunberg-Nissan	G_{12} = 0.71			24.11
	Hind *et al*	H_{12} = -4.26			19.42
	Katti-Chaudhri	W_{vis}/ RT=0.8			24.21
	Heric-Brewer (2-parameter)	α_{12} = 0.80	A_{21} = 0.01		24.11
	McAllister (3-body int)	Z_{12} = 25.56	Z_{21} = 11.97		42.64
	Lobe	α_{12} = 0.35	α_{21} = -1.01		25.92
	Heric-Brewer (3-parameter)	a = 1.72	b = -1.18	c = 0.93	53.88
	McAllister (4-body int)	Z_{1112} = 21.32	Z_{1122} = 11.6	Z_{1222} = 5.61	24.11
	Auslander	A_{21} = 0.56	B_{12} = 0.26	B_{21} = 0.93	24.09

Table 16
Coefficients of Jouyban- Acree model, mean relative deviation (MRD) and individual relative deviation (IRD) for liquid mixtures of 1,2-propanediol with2-PE/2-BE at various temperatures.

Temperature (K) 1,2-PD + 2-PE	J_0	J_1	J_2	MRD
p g.cm-3				
298.15	2.416	-0.107	0.019	0.0004
303.15	2.511	-0.110	0.013	0.0002
308.15	2.596	-0.114	0.015	0.0002
313.15	2.690	-0.117	0.038	0.0002
318.15	2.789	-0.127	0.024	0.0002
323.15	2.886	-0.133	0.022	0.0003
u m.s^{-1}				
298.15	1.009	1.132	1.473	0.0626
303.15	1.036	1.158	1.507	0.0630
308.15	1.064	1.184	1.542	0.0634
313.15	1.092	1.211	1.577	0.0638
318.15	1.120	1.238	1.613	0.0642
323.15	1.149	1.265	1.649	0.0646
n mPa.s				
298.15	3.306	0.016	-0.218	0.0006
303.15	3.589	-0.165	-0.236	0.0006
1,2-PD + 2-BE				
p g.cm^{-3}				
298.15	2.952	-0.138	-0.021	0.0002
303.15	3.060	-0.144	-0.002	0.0002
308.15	3.170	-0.141	-0.013	0.0003
313.15	3.282	-0.152	-0.013	0.0003
318.15	3.393	-0.158	-0.004	0.0003
323.15	3.508	-0.173	-0.022	0.0002
u m.s^{-1}				
298.15	0.342	0.609	0.559	0.0284
303.15	0.354	0.623	0.572	0.0286
308.15	0.366	0.637	0.586	0.0288
313.15	0.379	0.652	0.599	0.0290
318.15	0.392	0.666	0.612	0.0292
323.15	0.406	0.681	0.626	0.0294
n mPa.s				
298.15	3.133	-0.150	-0.036	0.0018
303.15	3.348	-0.165	-0.128	0.0013

7. Correlating models for viscosity

Several semi-empirical models [53–61] have been used to calculate the viscosities of the mixtures theoretically in terms of pure component values. The following semi-empirical models have been tested for the mixtures under study:

One parameter model

Grunberg-Nissan [55],

$$\ln\eta = x_1\ln\eta_1 + x_2\ln\eta_2 + x_1x_2G_{12} \tag{34a}$$

Hind, McLaughlin, and Ubbelohde [56],

$$\eta = x_1^2\ln\eta_1 + x_2^2\ln\eta_2 + 2x_1x_2H_{12} \tag{35a}$$

Katti and Chaudhri [57],

$$\ln(\eta V) = x_1\ln(\eta_1V_1) + x_2\ln(\eta_2V_2) + x_1x_2\frac{W_{vis}}{RT} \tag{36a}$$

Heric and Brewer [58,59]

$$\ln\nu = x_1\ln\nu_1 + x_2\ln\nu_2 + x_1\ln M_1 + x_2\ln M_2 - \ln(x_1M_1 + x_2M_2) + x_1x_2[\alpha_{12} + \alpha_{21}(x_1 - x_2)] \tag{37}$$

Two-parameter models

Lobe [60],

$$\nu = \phi_1\nu_1 e^{\phi_2\alpha_{12}\ln\left(\frac{\nu_2}{\nu_1}\right)} + \phi_2\nu_2 e^{\phi_1\alpha_{21}\ln\left(\frac{\nu_2}{\nu_1}\right)} \tag{38}$$

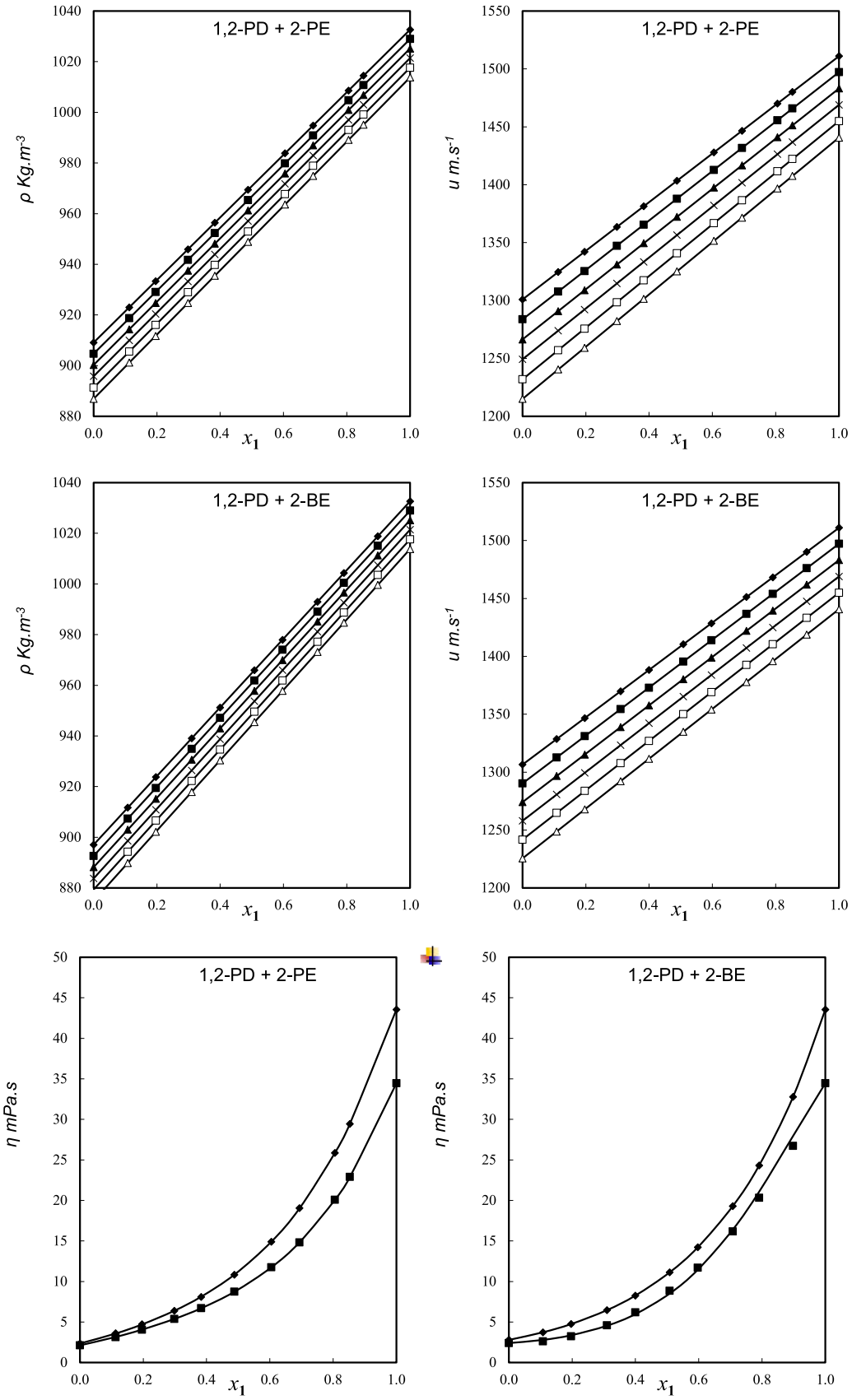

Fig 19. Plots of density (ρ), Speed of sound (u) and Viscosity(η) vs. mole fraction, x1 of 1,2-PD for 1,2-PD + 2-PE (or) +2-BE binary mixtures at temperatures, T/K = 298.15, ⁝; At T/K = 303.15, ■; T/K = 308.15, ▲; T/K = 313.15, ×; T/K = 318.15, □; T/K = 323.15, Δ. The points represent experimental values, and the lines represent values calculated from Eq. (43).

McAllister [61] (three-body interactions) model,

$$\ln\eta = x_1^3\ln\nu_1 + x_2^3\ln\nu_2 + 3x_1^2x_2\ln z_{12} + 3x_1x_2^2\ln z_{21} - \ln\left(x_1 + x_2\frac{M_2}{M_1}\right) - 3x_1^2x_2\ln\left(\frac{2}{3} + \frac{M_2}{3M_1}\right) + 3x_1x_2^2\ln\left(\frac{1}{3} + \frac{M_2}{3M_1}\right) - x_2^3\ln\left(\frac{M_2}{M_1}\right) \quad (39)$$

McAllister [61,62] (four-body interactions) model,

$$\ln\nu - \left(x_1^4\ln\nu_1 + x_2^4\ln\nu_2\right) = 4x_1^3x_2\ln z_{1112} + 6x_1^2x_2^2\ln z_{1122} + 4x_1x_2^3\ln z_{1222} - \ln\left(x_1 + x_2\frac{M_2}{M_1}\right) + 4x_1^3x_2\ln\left(\frac{3}{4} + \frac{M_2}{4M_1}\right) + 6x_1^2x_2^2\ln\left(\frac{1}{2} + \frac{M_2}{2M_1}\right) + 4x_1x_2^3\ln\left(\frac{1}{4} + \frac{3M_2}{4M_1}\right) + x_2^4\ln\left(\frac{M_2}{M_1}\right) \quad (40)$$

Heric and Brewer [58,59]

$$\ln\nu = x_1\ln\nu_1 + x_2\ln\nu_2 + x_1\ln M_1 + x_2\ln M_2 - \ln(x_1M_1 + x_2M_2) + x_1x_2\left[a + b(x_1 - x_2) + c(x_1 - x_2)^2\right] \quad (41)$$

Three-parameter model,

Auslander [56,63] model

$$\eta = \frac{\eta_1x_1(x_1 + B_{12}x_2) + \eta_2x_1[(A_{21}x_2(B_{21}x_1 + x_2)]}{(x_1 + B_{12}x_2) + [(A_{21}x_2(B_{21}x_1 + x_2)]} \quad (42)$$

From Table 15, empirical and semi-empirical models (1,2, and 3-parameter models) fitting and APD were presented at 298.15 and 303.15 K. The comparison of viscosity models for 2-propoxyethanol & 2-butoxyethanol at 298.15 K and 303.15 K reveals significant deviation variations. Heric-Brewer (2-parameter) performed best with 1.41% (2-propoxy) and 4.34% (2-butoxy), while Heric-Brewer (3-parameter) and McAllister (3-body int) had the highest deviations, reaching 53.88%. Although the 3-body model captures fundamental interactions, the McAllister 4-body model proved superior by incorporating higher-order molecular effects and hydrogen bonding, resulting in lower deviations and better accuracy. Lobe and Auslander models showed the lowest deviations, ensuring reliability. Grunberg-Nissan and Katti-Chaudhri exhibited moderate performance. Higher temperatures worsened deviations, particularly for McAllister (3-body int) at 42.64% (2-butoxy). The graph visually compares model performances, highlighting the most and least accurate predictions. The graphical comparison was given as Fig 6S (*Supplementary Information*)

Jouyban – Acree Model

The Jouyban–Acree model is an empirical correlation widely used to predict physicochemical properties of binary liquid mixtures, such as density, Speed of Sound and Viscosity as a function of composition and temperature. This model combines the contributions of the pure components with an interaction term that accounts for non-ideal behaviour in mixtures. The general form of the model expresses the natural logarithm of a mixture property (eg, density) as a function of the mole fractions of the components, the properties of the pure substances, and a polynomial interaction term that captures non-ideal behaviour. The interaction term is a polynomial expansion scaled by the temperatures. Specifically, this model is represented as [65]

$$\ln P_{mix,T} = x_1\ln P_1 + x_2\ln P_2 + \frac{x_1x_2}{T}\left(J_0 + J_1(x_1 - x_2) + J_2(x_1 - x_2)^2\right) \quad (43)$$

Where $P_{mix,T}$ is the property of the mixture at temperature T, x_1 and x_2 are the mole fractions, P_1 and P_2 are the pure components, and J_0, J_1 and J_2 are empirical coefficients obtained by regressions. This model is valued for its simplicity, flexibility and applicability across various thermophysical properties and binary mixtures.

In this study, the model was successfully applied to predict density, speed of sound and Viscosity for the binary mixtures of 1,2-PD with 2-PE & 2-BE. The fitted J coefficients (Table 16) provided excellent agreement between experimental and predicted values, with Mean Relative Deviations (MRD) typically within 0.1-0.8%. The experimental and predicted density, speed of sound and Viscosity were graphically represented in Fig. 19.

8. Conclusions

The density (p) and speed of sound (u) for binary mixtures of propylene glycol (1,2-PD) with ether alcohols were measured over T=298.15-323.15 K, and viscosity (n) was measured at T=298.15 and 303.15 K. Results showed that increasing chain length decreases density while increasing the speed of sound, and both properties decrease with rising temperature. Excess and deviation properties, along with partial molar properties at infinite dilution, provided insights into molecular interactions, indicating dominant hydrogen bonding and dipole-dipole interactions. The PC-SAFT model effectively predicted density (0.65% deviation) and speed of sound (0.20% deviation when coupled with SCFT) without fitted parameters. Viscosity was modelled using FVT + PC-SAFT with a deviation of 1.23%. Negative values of excess properties, becoming more negative with temperature, reflect strong molecular interactions. Heric-Brewer (2-parameter), Lobe, and Auslander models offer the most accurate viscosity predictions, while McAllister (3-body) and Heric-Brewer (3-parameter) show the highest deviations, worsening at higher temperatures. These findings highlight the suitability of PC-SAFT and coupled models (SCFT, NR, and FVT) for accurately modelling the thermophysical properties of the investigated binary mixtures. The MRD of the Jouyban-Acree model within the limits 0.1-0.8% and predicted the density, SOS and Viscosity well.

CRediT authorship contribution statement

Subhasri Ganji: Formal analysis. **Ariel Hernández:** Software. **T.S. Krishna:** Writing – original draft, Validation, Investigation, Formal analysis, Data curation, Conceptualization. **Ranjan Dey:** Writing –

original draft. **D. Ramachandran:** Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.ctta.2025.100213.

Data availability

No data was used for the research described in the article.

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