Comparative Ultrasonic and Acoustic Properties of Ethylbenzoate with Secondary and Tertiary Butanol Binary Mixtures

LakshmanaRao G[1], Suresh P [2*], Beebi SK[2]

[1]Dept. of Chemistry, Dr. V. S. Krishna Govt. Degree College(A), Visakhapatnam, A.P., India.

[2] Dept. of Chemistry, SRR & CVR Govt. Degree College(A), Vijayawada, A.P., India.

***Corresponding Author**

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ABSTRACT

This work reports on the ultrasonic velocity, density, viscosity, and derived acoustic parameters of binary mixtures of ethylbenzoate with 2-butanol and 2-methyl-2-propanol over a range of compositions at 303.15 K, 308.15 K, 313.15 K, and 318.15 K. The experimental measurements were used to calculate adiabatic compressibility, intermolecular free length, internal pressure, and acoustic impedance to elucidate underlying molecular interactions. For both systems, increasing ethylbenzoate mole fraction produced higher velocity and density, and lower viscosity and compressibility, indicating enhanced structural ordering. The ethylbenzoate + 2-butanol system exhibited stronger cohesive interactions, as revealed by higher ultrasonic velocities, acoustic impedance and internal pressure compared to the ethylbenzoate + 2-methyl-2-propanol system, attributed to reduced steric hindrance and more effective hydrogen bonding in the former. Temperature elevation weakened interactions in both mixtures, consistent with increased thermal agitation. These findings are significant for designing solvent systems in chemical processing and provide fundamental insights into mixture behavior relevant to industrial and environmental applications.

Keywords: Ultrasonic velocity, adiabatic compressibility, internal pressure, binary mixtures, acoustic impedance, intermolecular interactions.

INTRODUCTION

Binary liquid mixtures exhibit complex behaviour driven by intermolecular interactions such as hydrogen bonding, dipole–dipole forces, and dispersion effects. Ultrasonic velocity and related acoustic parameters have been widely used to probe such interactions because they reflect changes in molecular packing and cohesion [1]–[4]. Ultrasonic techniques offer precision for determining physical properties like adiabatic compressibility (βad), acoustic impedance (Z), and internal pressure (π), which correlate with interaction strength and structural organization in liquids [5]–[8].

Alcohol–ester mixtures have attracted significant interest due to their relevance in chemical synthesis, solvent design, and industrial applications where miscibility and transport properties are critical [9]–[12]. Prior studies have shown that secondary alcohols generally form stronger hydrogen bonding compared to tertiary alcohols due to lower steric hindrance around the hydroxyl group [13]–[18]. Similarly, the introduction of bulky substituents is known to disrupt cohesive forces and lead to structure-breaking behaviour [19]–[22].

Despite extensive literature on alcohol–ester mixtures, comparative studies focusing on ethylbenzoate with structurally distinct alcohols remain limited, particularly at multiple temperatures. The current work addresses this gap by experimentally evaluating the ultrasonic and acoustic properties of ethylbenzoate mixed with 2-butanol and 2-methyl-2-propanol. The influence of molecular structure on interaction strength is analyzed through a series of measured and derived parameters across four temperatures.

MATERIALS AND METHODS

Materials

Ethylbenzoate (≥99 % purity), 2-butanol (≥99 %) and 2-methyl-2-propanol (≥99 %) were obtained from commercial suppliers and used without further purification. All liquids were dried and stored over molecular sieves to minimize water content.

B. Preparation of Mixtures

Binary mixtures of ethylbenzoate (X_1) with each alcohol (X_2) were prepared gravimetrically in mole fractions ranging from 0.0000 to 1.0000. Samples were equilibrated at target temperatures (303.15 K – 318.15 K) in a thermostated water bath (±0.05 K accuracy).

Measurements

Ultrasonic velocities were measured using a digital ultrasonic interferometer (±0.1 m/s precision). Densities were obtained via a vibrating-tube densitometer ($\pm 0.0001\ g\cdot cm^{-3}$), and viscosities via a Ubbelohde viscometer (±0.5 % accuracy). Adiabatic compressibility, internal pressure, acoustic impedance, free length and molar volume were calculated using standard thermodynamic relations [23]–[25].

RESULTS AND DISCUSSION

A. Ultrasonic Velocity and Density

Ultrasonic velocity increased with ethylbenzoate mole fraction for both systems at all temperatures, indicative of stronger cohesive forces and reduced free volume [6], [16]. The ethylbenzoate + 2-butanol mixture consistently exhibited higher velocities and densities than the ethylbenzoate + 2-methyl-2-propanol mixture at equivalent compositions, reflecting more effective molecular packing due to lower steric hindrance in 2-butanol.

B. Viscosity and Derived Acoustic Parameters

Viscosity decreased with increasing temperature and ethylbenzoate content, aligning with reduced hydrogen bonding at elevated temperatures [10], [14]. The ethylbenzoate + 2-methyl-2-propanol system showed slightly higher viscosities at low X_1, likely due to the bulkier tertiary alcohol causing structural constraints.

Derived parameters such as adiabatic compressibility and intermolecular free length decreased with ethylbenzoate content, confirming stronger interactions [7], [24]. Internal pressure and acoustic impedance followed opposite trends, increasing with ethylbenzoate mole fraction and underscoring enhanced cohesion in 2-butanol mixtures.

C. Temperature Effects

All measured and calculated properties exhibited systematic temperature dependence: rising temperature led to lower velocity, density, internal pressure and higher free length. These trends illustrate thermal disruption to structured interaction networks [5], [20].

Table 1 Ethylbenzoate(X1) + 2-butanol(X2) Ultrasonic velocities, Densities, Viscosities and related Acoustic Parameters

X_1	U (m/s)	$\rho \times 10^{-3}$ (g/cm^3)	η (cP)	V (cm^3/mol)	$\beta ad \times 10^{-12}$ (m^{2}N^{-1})	Lf (Å)	π (Nm^{-2})	Z (kg m^{-2} s^{-1})	H (J/mol)
0.0000	1152.0	798.20	2.595	92.859	16.626	0.8092	9.0122	919.53	836.866
0.0666	1171.1	823.70	2.537	96.137	16.650	0.8098	8.3550	964.64	803.224
0.1384	1190.7	849.70	2.474	99.619	16.685	0.8107	7.7287	1011.74	769.925

0.2159	1210.7	876.00	2.407	103.358	16.733	0.8118	7.1325	1060.57	737.197
0.2999	1231.1	902.40	2.335	107.412	16.795	0.8133	6.5626	1110.94	704.901
0.3912	1251.6	928.70	2.257	111.846	16.868	0.8151	6.0170	1162.36	672.974
0.4908	1272.1	954.50	2.173	116.758	16.954	0.8172	5.4939	1214.22	641.465
0.5999	1292.3	979.30	2.082	122.274	17.053	0.8196	4.9914	1265.55	610.312
0.7199	1311.8	1002.40	1.982	128.561	17.167	0.8223	4.5062	1314.95	579.320
0.8526	1330.1	1022.60	1.873	135.888	17.301	0.8255	4.0374	1360.16	548.635
1.0000	1346.2	1039.20	1.751	144.505	17.439	0.8288	3.5827	1398.97	517.723
0.0000	1142.5	793.30	2.150	93.432	16.454	0.8050	8.2035	906.35	766.471
0.0666	1161.0	819.20	2.108	96.665	16.454	0.8050	7.6211	951.09	736.691
0.1384	1180.0	845.40	2.066	100.126	16.470	0.8054	7.0707	997.57	707.960
0.2159	1199.4	871.60	2.021	103.880	16.505	0.8063	6.5443	1045.40	679.820
0.2999	1219.1	898.10	1.974	107.926	16.548	0.8073	6.0444	1094.87	652.344
0.3912	1239.0	924.60	1.922	112.342	16.603	0.8087	5.5642	1145.58	625.096
0.4908	1259.0	950.40	1.867	117.262	16.678	0.8105	5.1042	1196.55	598.530
0.5999	1278.7	975.30	1.808	122.775	16.765	0.8126	4.6633	1247.12	572.533
0.7199	1297.9	998.50	1.743	129.063	16.871	0.8152	4.2373	1295.95	546.882
0.8526	1315.8	1018.70	1.673	136.408	16.995	0.8182	3.8267	1340.41	521.991
1.0000	1331.9	1034.80	1.596	145.120	17.143	0.8217	3.4291	1378.25	497.628
0.0000	1137.5	789.50	1.734	93.882	16.389	0.8034	7.4792	898.06	702.165
0.0666	1155.0	815.60	1.709	97.092	16.356	0.8026	6.9709	942.02	676.822
0.1384	1172.9	841.90	1.686	100.542	16.340	0.8022	6.4927	987.46	652.790
0.2159	1191.2	868.30	1.663	104.275	16.342	0.8023	6.0382	1034.32	629.631
0.2999	1209.9	894.80	1.637	108.324	16.360	0.8027	5.6011	1082.62	606.730
0.3912	1228.7	921.00	1.612	112.781	16.392	0.8035	5.1866	1131.63	584.952
0.4908	1247.5	946.70	1.584	117.720	16.439	0.8047	4.7873	1181.01	563.559
0.5999	1266.1	971.40	1.555	123.268	16.502	0.8062	4.4049	1229.89	542.984
0.7199	1284.1	994.70	1.524	129.556	16.577	0.8080	4.0378	1277.29	523.119
0.8526	1301.0	1014.90	1.491	136.919	16.678	0.8105	3.6828	1320.38	504.245
1.0000	1316.0	1030.60	1.455	145.711	16.804	0.8136	3.3382	1356.27	486.414
0.0000	1132.8	785.50	1.395	94.360	16.337	0.8022	6.8065	889.81	642.267
0.0666	1149.2	812.20	1.384	97.498	16.260	0.8003	6.3716	933.38	621.225
0.1384	1165.9	838.60	1.376	100.938	16.209	0.7990	5.9614	977.72	601.730
0.2159	1183.1	864.80	1.371	104.697	16.186	0.7984	5.5741	1023.14	583.585
0.2999	1200.5	891.10	1.366	108.774	16.173	0.7981	5.2041	1069.77	566.069
0.3912	1218.1	917.10	1.362	113.261	16.179	0.7983	4.8509	1117.12	549.416
0.4908	1235.6	942.80	1.357	118.207	16.193	0.7986	4.5109	1164.92	533.224
0.5999	1252.9	967.50	1.354	123.765	16.225	0.7994	4.1867	1212.18	518.166
0.7199	1269.6	990.60	1.350	130.093	16.272	0.8006	3.8723	1257.67	503.754
0.8526	1285.2	1010.70	1.349	137.488	16.343	0.8023	3.5709	1298.95	490.955
1.0000	1299.0	1026.00	1.348	146.365	16.446	0.8048	3.2759	1332.77	479.480

Table 2 Ethylbenzoate(X1) + 2-methyl-2-propanol(X2) Ultrasonic velocities, Densities, Viscosities and related Acoustic Parameters

Mole fraction X_1	**Velocity (U) m/s**	**Density $(\rho)X10^{-3}$ gm/cm^3**	**Viscosity (η) cP**	**Mol.Vol. V cm^3 mol^{-1}**	**Ad. Comp. $\beta_{ad}\times10^{-12}$ m^{2}N^{-1}**	**Int Mol. Free Length $L_{f\,(Å)}$**	**internal pressure π Nm^{-2}**	**Acoustic impedance (Z) Kg m^{-2} s^{-1}**	**Enthalpy H Jmol^{-1}**
					303.15K				
0.0000	1061.0	775.30	3.3720	95.6017	14.5198	0.7562	10.50	822.59	1003.72
0.0685	1087.8	806.20	3.2580	98.3969	14.6776	0.7603	9.66	876.98	950.95

0.1419	1115.4	837.10	3.1360	101.4373	14.8622	0.7651	8.87	933.70	899.62
0.2209	1143.7	868.10	3.0060	104.7339	15.0680	0.7704	8.11	992.85	849.60
0.3061	1172.6	898.70	2.8670	108.3744	15.2998	0.7763	7.39	1053.82	800.79
0.3982	1202.0	928.40	2.7170	112.4518	15.5623	0.7829	6.70	1115.94	752.90
0.4981	1231.7	956.90	2.5550	117.0439	15.8542	0.7902	6.03	1178.61	705.71
0.6069	1261.4	983.30	2.3790	122.3151	16.1815	0.7983	5.39	1240.33	658.95
0.7258	1290.8	1006.70	2.1890	128.4527	16.5508	0.8074	4.77	1299.45	612.53
0.8562	1319.3	1025.00	1.9810	135.7191	16.9661	0.8175	4.17	1353.47	565.74
1.0000	1346.2	1039.20	1.7510	144.5054	17.4389	0.8288	3.58	1398.97	517.72
					308.15K				
0.0000	1055.7	770.10	2.5890	96.2472	14.4722	0.7550	9.18	812.99	883.68
0.0685	1081.5	801.40	2.5150	98.9862	14.5950	0.7582	8.48	866.71	839.61
0.1419	1108.1	832.70	2.4390	101.9733	14.7458	0.7621	7.82	922.71	797.38
0.2209	1135.3	864.00	2.3590	105.2309	14.9179	0.7665	7.19	980.90	756.60
0.3061	1163.2	894.90	2.2730	108.8346	15.1194	0.7717	6.59	1040.95	716.91
0.3982	1191.6	924.90	2.1810	112.8774	15.3520	0.7776	6.01	1102.11	678.35
0.4981	1220.3	953.50	2.0810	117.4613	15.6175	0.7843	5.45	1163.56	640.62
0.6069	1249.1	979.90	1.9740	122.7395	15.9226	0.7919	4.92	1223.99	603.89
0.7258	1277.6	1003.20	1.8590	128.9008	16.2706	0.8005	4.41	1281.69	568.04
0.8562	1305.5	1022.10	1.7340	136.2236	16.6748	0.8104	3.91	1334.35	532.75
1.0000	1331.9	1034.80	1.5960	145.1198	17.1430	0.8217	3.43	1378.25	497.63
					313.15K				
0.0000	1047.6	764.80	2.0460	96.9142	14.3497	0.7518	8.29	801.20	803.24
0.0685	1072.6	796.40	1.9990	99.6077	14.4459	0.7543	7.68	854.22	765.43
0.1419	1098.3	828.10	1.9520	102.5397	14.5666	0.7575	7.11	909.50	729.49
0.2209	1124.7	859.70	1.9020	105.7573	14.7139	0.7613	6.57	966.90	694.80
0.3061	1151.7	890.90	1.8500	109.3232	14.8885	0.7658	6.05	1026.05	661.53
0.3982	1179.2	921.10	1.7950	113.3430	15.0962	0.7711	5.55	1086.16	629.53
0.4981	1207.1	949.80	1.7360	117.9189	15.3410	0.7773	5.08	1146.50	598.62
0.6069	1235.2	976.30	1.6720	123.1921	15.6276	0.7846	4.62	1205.93	568.67
0.7258	1263.0	999.60	1.6050	129.3651	15.9581	0.7928	4.18	1262.49	540.11
0.8562	1290.1	1018.30	1.5340	136.7320	16.3445	0.8023	3.75	1313.71	512.88
1.0000	1316.0	1030.60	1.4550	145.7112	16.8043	0.8136	3.34	1356.27	486.41
					318.15K				
0.0000	1038.1	760.00	1.6890	97.5263	14.1796	0.7473	7.65	788.96	746.41
0.0685	1062.3	792.00	1.6570	100.1610	14.2485	0.7491	7.12	841.34	712.75
0.1419	1087.1	823.90	1.6270	103.0624	14.3438	0.7516	6.61	895.66	681.26
0.2209	1112.7	855.80	1.5970	106.2392	14.4672	0.7549	6.13	952.25	651.29
0.3061	1138.9	887.20	1.5660	109.7792	14.6201	0.7588	5.67	1010.43	622.68
0.3982	1165.6	917.50	1.5330	113.7878	14.8079	0.7637	5.23	1069.44	595.28
0.4981	1192.7	946.30	1.4990	118.3550	15.0326	0.7695	4.81	1128.65	569.24
0.6069	1220.0	972.80	1.4630	123.6353	15.3002	0.7763	4.40	1186.82	544.44
0.7258	1247.1	995.90	1.4250	129.8457	15.6166	0.7843	4.01	1241.99	520.98
0.8562	1273.6	1014.30	1.3860	137.2712	15.9919	0.7936	3.64	1291.81	499.15
1.0000	1299.0	1026.00	1.3430	146.3645	16.4464	0.8048	3.27	1332.77	478.59

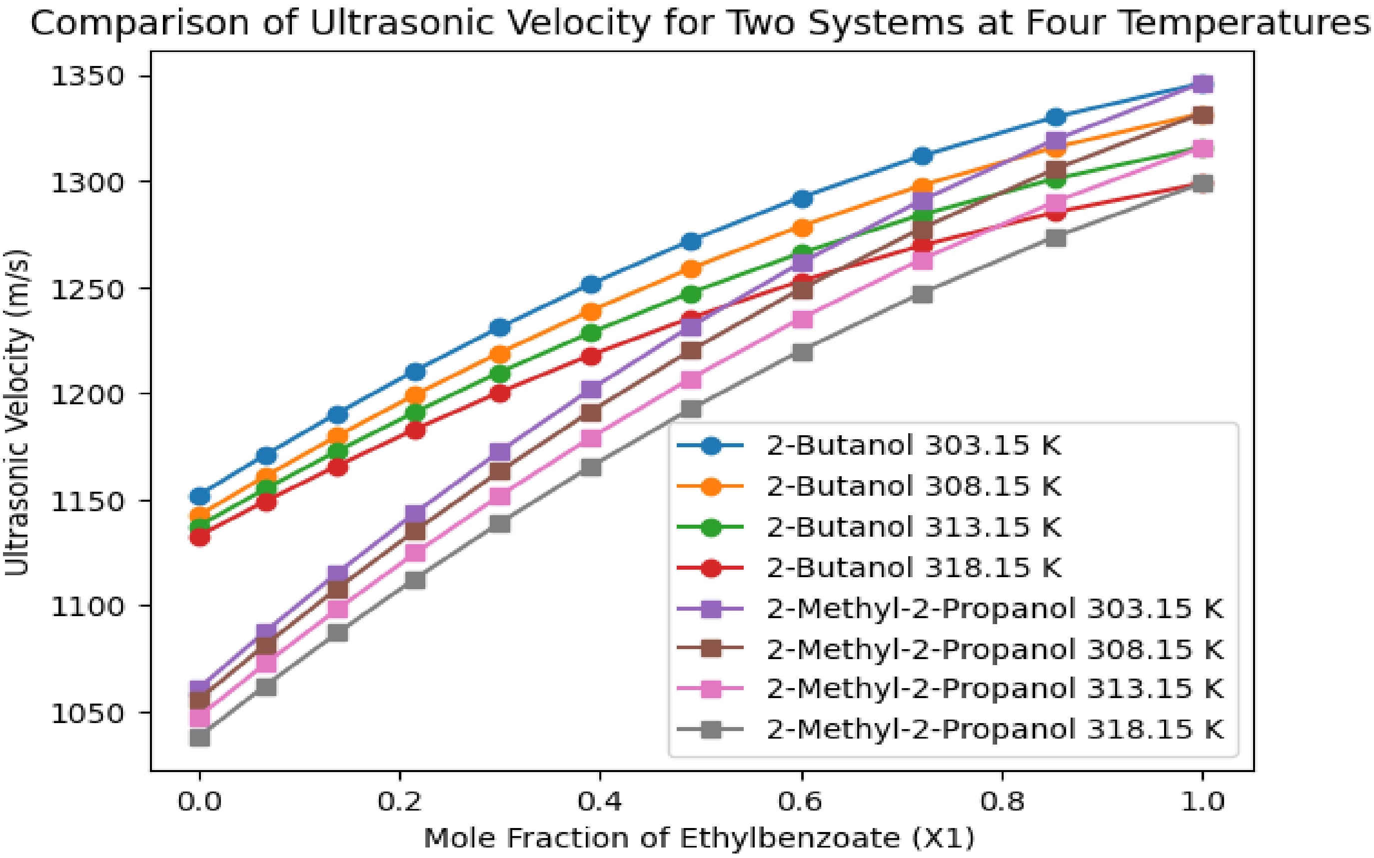

Figure-1 Comparison of Ultrasonic velocity for two systems

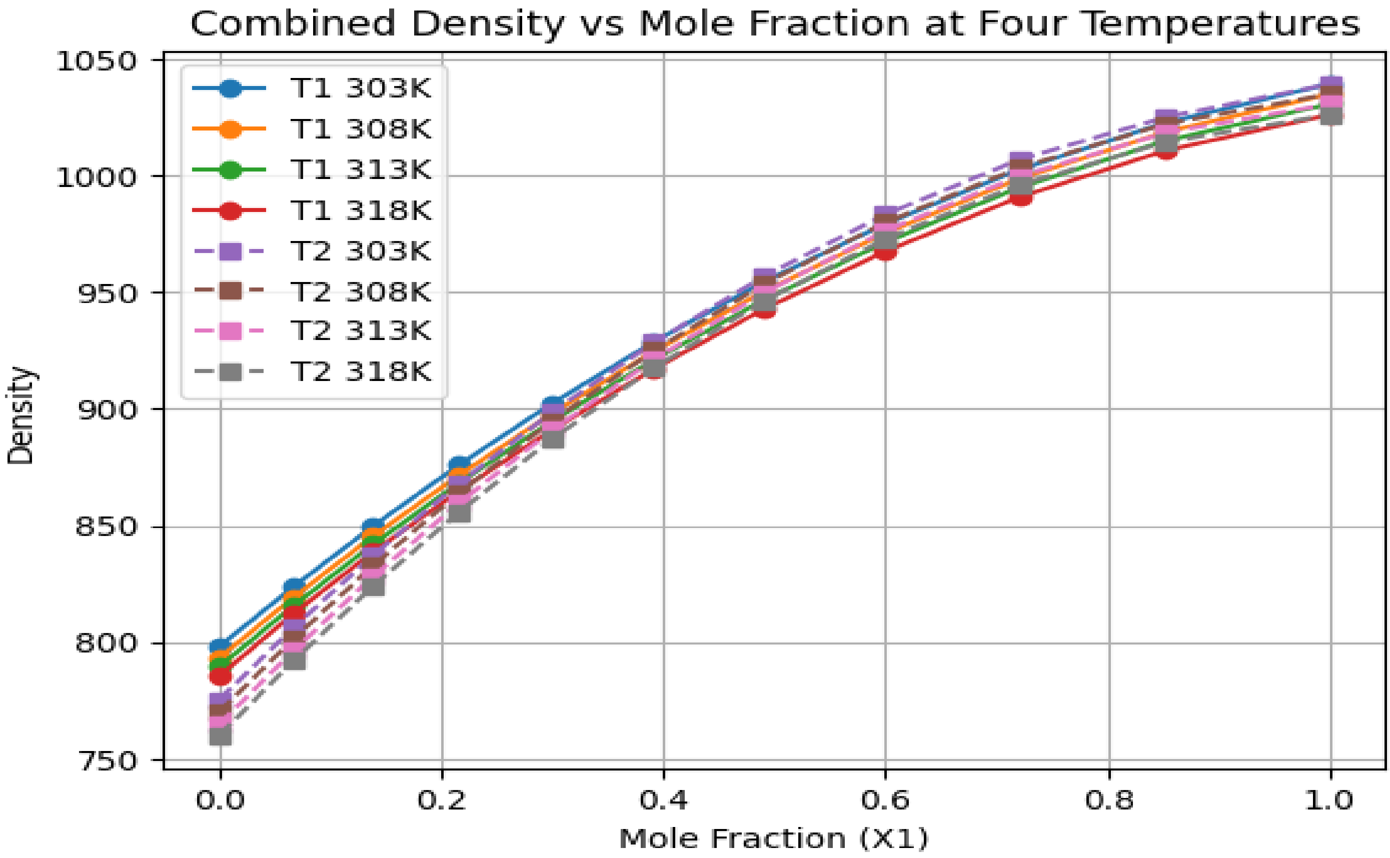

Figure-2. Comparative Density of Two systems at four temperatures

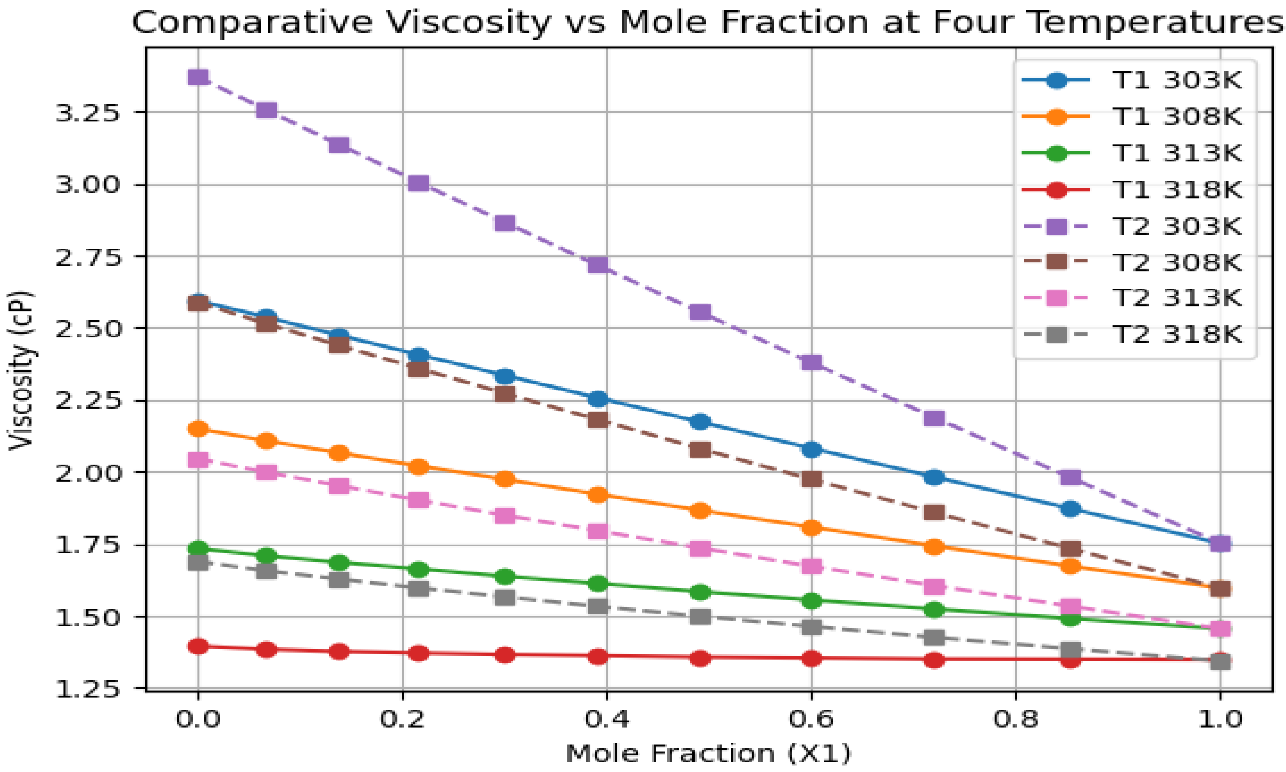

Figure-4. Comparative viscosity for two systems at four temperatures

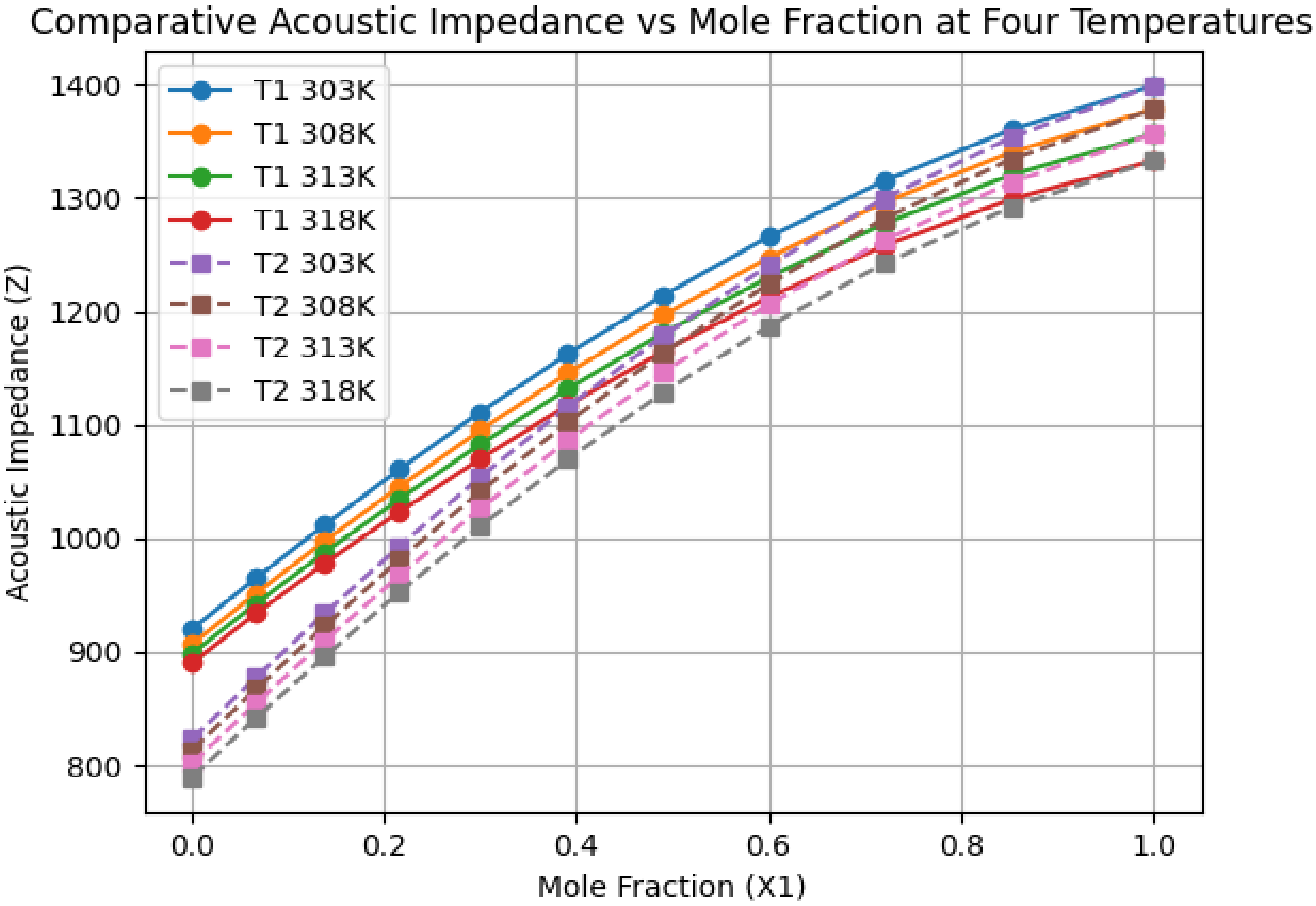

Figure-5. Comparative Acoustic Impedance for two systems at four temperatures

CONCLUSION

The present investigation provides a comprehensive and comparative analysis of the thermo-acoustic behaviour of ethylbenzoate when mixed with structurally distinct alcohols, namely 2-butanol and 2-methyl-2-propanol, over a wide temperature range. The systematic variation of ultrasonic velocity, density, viscosity, and derived acoustic parameters clearly demonstrates that intermolecular interactions in these binary systems are highly sensitive to both molecular structure and temperature.

The observed increase in ultrasonic velocity, acoustic impedance, and internal pressure, along with the decrease in adiabatic compressibility and intermolecular free length with increasing ethylbenzoate concentration, confirms the progressive enhancement of cohesive forces and structural compactness in the mixtures. Among the two systems, the ethylbenzoate + 2-butanol mixture exhibits significantly stronger associative interactions compared to the ethylbenzoate + 2-methyl-2-propanol system. This is primarily attributed to reduced steric hindrance and greater accessibility of the hydroxyl group in 2-butanol, facilitating more effective hydrogen bonding and dipole–dipole interactions with the ester functional group. In contrast, the bulky tertiary structure of 2-methyl-2-propanol restricts interaction efficiency, leading to weaker cohesion and partial structural disruption.

The influence of temperature further substantiates these findings, as increased thermal energy consistently weakens intermolecular associations, resulting in reduced structural ordering across both systems. This highlights the delicate balance between molecular forces and thermal agitation in determining liquid structure.

From an industrial perspective, these findings hold significant relevance in the rational design and optimization of solvent systems. The stronger interaction and better structural stability observed in the ethylbenzoate + 2-butanol system make it a more suitable candidate for applications requiring enhanced solute–solvent interactions, such as extraction processes, reaction media in organic synthesis, and formulation of coatings, fragrances, and pharmaceuticals. Conversely, the weaker interactions in the ethylbenzoate + 2-methyl-2-propanol system may be advantageous in processes where lower viscosity, reduced association, and easier molecular mobility are desired, such as in fuel blending, cleaning formulations, and diffusion-controlled systems.

Overall, this study establishes a clear correlation between molecular architecture and macroscopic acoustic behaviour, offering valuable insights for tailoring liquid mixtures with desired physicochemical properties. The results contribute not only to the fundamental understanding of intermolecular interactions but also provide a practical framework for selecting appropriate solvent combinations in diverse chemical and industrial applications.

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