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Theoretical evaluation of ultrasonic velocity in binary mixtures of alkanols with di ethyl malonate

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ABSTRACT

Nomoto's relation, ideal mixing relation (IMR) impedance dependence relation (IDR), Rao's velocity method (RVM) and Junjie's method (JM) were used for evaluating the theoretical values of ultrasonic velocity in binary liquid mixtures of diethyl malonate (DEM) + 1- butanol, di ethyl malonate (DEM) + pentanol and di ethyl malonate (DEM) + hexanol at 303.15,308.15,313.15 and 318.15K. The relative merits of these theoretical relations were examined by comparing the theoretical values of ultrasonic velocity with the values obtained experimentally. The validity of the theories was checked by applying the chi-square test for goodness of fit and by calculating the average percentage error (APE).

KEYWORDS

Ultrasonic velocity;
Di ethyl malonate;
1- alkanols;
Chi-square test.

INTRODUCTION

Thermodynamic and thermo acoustical properties are the most important parameters to characterize the physicochemical behaviour of a binary or ternary systems leading to interpretation of the molecular interactions taking place between them. Measurement of ultrasonic velocity[1-5] has been adequately employed in understanding the molecular interactions in pure, binary, and higher order multi component liquid mixtures. The propagation of ultrasonic velocity in a medium is a thermodynamic property and has come to be recognized as a very specific and unique tool for predicting and estimating various physico -chemical properties of the systems under consideration. A sound wave is a pressure wave and can be treated as a series of compressions and rarefactions travelling along a material so that the molecular planes are displaced from their mean positions. It is assumed that these compressions and rarefactions are reversible and adiabatic. Since ultrasonic velocity data proves to be a very simple and convenient tool to determine various thermodynamic properties of liquid and liquid mixtures, significant amount of work has been done in carrying out investigation pertaining to various thermodynamic, physicochemical and liquid state properties by using ultrasonic velocity in conjunction with density. Scarcity of data on ternary and higher multi component liquid mixtures led us to the present investigation.

Theoretical evaluation of ultrasonic velocity in

binary liquid mixtures and its comparison with the experimental values reflects the molecular interaction in liquid mixtures, which is very useful to build comprehensive theoretical model for liquids. Several researchers[6-9] carried out investigations on liquid mixtures and correlated the experimental results of ultrasonic velocity with the theoretical relations like Nomoto's relation[10], ideal mixing relation (IMR)[11], impedance dependence relation (IDR)[12], Rao's velocity method (RVM)[13] and Junjie's method (JM)[14].

In the present investigation di ethyl malonate is mixed with 1- alkanols at different mole fractions to study the interactions between the component molecules. The results are explained and discussed in terms of molecular interactions in the investigated systems. Further, the best suitable theory for the given studied systems for evaluating theoretical velocities is also picked out by computing the average percentage error and Chi-Square test.

The deviation in the variation of U^2_{exp}/ U^2_{imx}, standard deviation, Chi-square test for goodness of fit from unity have also been evaluated to further explain the non-ideality of the system. The ratio of $U_{exp}{}^{2}/U_{imx}{}^{2}$ gives an idea of extent of interaction taking place between molecules of the mixtures, positive values of which infer strong interactions between the components.

EXPERIMENTAL

Di ethyl malonate, 1-butanol 1-pentanol and 1-hexanol from Merk were purified as described in the literature[15,16]. The pure chemicals were stored over activated 4Å molecular sieves to reduce water content before use.

All the binary liquid mixtures are prepared by weighing an amount of pure liquids in an electric balance (Afoset, ER-120A, and India) with a precision of ±0.1 mg by syringing each component into air-tight stopper bottles to minimize evaporation losses. The uncertainty on mole fraction is estimated to be $1x10^{-4}$. It is ensured that the mixtures are properly mixed and the measurement of the required parameters was done within one day of preparation.

The densities, ρ, of pure liquids and their mixtures are determined using a 10^{-5} m^3 double-arm pycnometer, and the values from triplicate replication at each temperature are reproducible within 2×10^{-1} kg m^3 and the uncertainty in the measurement of density is found to be 2 parts in 10^4 parts. The reproducibility in mole fractions was within ±0.0002

Temperature control for the measurement of viscosity and density is achieved by using a microprocessor assisted circulating water bath, (supplied by Mac, New Delhi) regulated to ±0.01 K, using a proportional temperature controller. Adequate precautions were taken to minimize evaporation losses during the actual measurements.

The ultrasonic velocity of sound (U) is measured using an ultrasonic interferometer (Mittal Enterprises, New Delhi model F05) operating at 2 MHz. The measured speeds of sound have a precision of 0.8 $m.sec^{-1}$ and an uncertainty less than ± 0.1 $m.sec^{-1}$. The temperature stability was maintained within±0.01K. by circulating water bath around the measuring cell through a pump.

THEORETICAL CONIDERATIONS

Nomoto equation

The ratio of temperature coefficients of sound velocity U and molar volume V remains almost constant for pure liquids[17].

$$[(1/U)\,(dU/dT)] / [(1/V)\,(dV/dT)] = -3 \quad (1)$$

where T is the absolute temperature.

Integration the above equation, we get

$$VU^{1/3} = const = M/\rho U^{1/3} = R \quad (2)$$

Where U and ρ are determined experimentally and M is the mean molecular weight in a binary liquid mixture

$$M = (X_1M_1 + X_2M_2) \quad (3)$$

where M_1 and M_2 are molecular weights of constituent components.

Simple manipulation yields the following relation

$$U_{Nomoto} = [(X_1R_1+X_2R_2) / (X_1V_1+X_2V_2)]^3 \quad (4)$$

The Van Dael and Vangeel Equation

Van Dael[11] obtained the relation for ultrasonic velocity in liquid mixtures as

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$$1/(X_1M_1+X_2M_2)*1/U^2_{imx} = X_1/M_1U_1^2 + X_2/M_2U_2^2 \quad (5)$$

where U_{imx} is the ideal mixing ultrasonic velocity in liquid mixture. U_1 and U_2 are ultrasonic velocities in species.

The impedance relation

$$\text{Impedance relation } U = \Sigma X_i Z_i / \Sigma X_i\rho_I \quad (6)$$

where X_i mole fraction, $\rho_{t,}$ is the density of the mixture and Z_i is the acoustic impedance.

The Rao's Specific Velocity Method Relation

$$\text{Rao's specific velocity method}[13]\ U = (\Sigma X_i r_i \rho)^3 \quad (7)$$

where X_i mole fraction, U_i is the ultrasonic velocity, ρ_t is the density of the mixture, r_i is the Rao's specific sound velocity = $Ui^{1/3}/\rho_i$ and Z_i is the acoustic impedance.

The junjie equation

$$U_J = (X_1M_1/\rho_1+X_2M_2/\rho_2)/[\{X_1M_1+X_2M_2\}^{1/2}$$
$$\{X_1M_1/\rho_1U_1^2+X_2M_2/\rho_2U_2^2)\}^{1/2}] \quad (8)$$

where M_1, M_2 are molecular weights of constituent components.. ρ_1 and ρ_2 are the densities of constituent components.

Chi-square test for goodness of fit

According to Karl Pearson[18] Chi-square value is evaluated for the binary liquid mixtures under study using the formula

$$\chi^2 = \sum_{i=1}^{N} (U_{mix(obs)} - U_{mix(cal)})^2 / U_{mix(cal)} \quad (9)$$

where n is the number of data used.

Average percentage error (APE)

The Average percentage error[19] calculated using the relation

$$APE = 1/n \Sigma (Umix(obs) - Umix(cal)) / Umix(obs)) X100\% \quad (10)$$

where n is the number of data used.

$U_{mix(obs)}$ = experimental values of ultrasonic velocities

$U_{mix(cal)}$ = computed values of ultrasonic velocities

DISCUSSIONS

Alkanols are self associated liquids with hydrogen bond between them. This Self association decreases with increasing chain length in their pure state. When alkanols are mixed with diethyl malonate, there will be an interaction between their individual functional groups (OH and C=O) through the formation of hydrogen bond.

The experimental values of ultrasonic velocity for the system along with theoretical values and percentage deviations for Nomoto's Relation (U_{NR}), Vandeal Vangael Ideal Mixing Relation (U_{imx}), Impedance Dependence Relation (U_I), Rao's specific velocity method (U_{Rao}) and Junjie's relation (U_J) are compared for all the three binaries. The agreement between theoretical velocities of Nomoto's relation in Dem + 1- Hexanol system suggests that R is additive property in all the three systems. It is observed that the experimental values show deviation with the theoretical values of ultrasonic velocities which confirms the existence of molecular interactions.

TABLES 1, 2, and 3 show the values of ultrasonic velocity computed by various theories along with experimental values (U) and percentage of deviations. There are variations between the evaluated and experimental values. From the observed values of all three systems, there is a good agreement between theoretical and experimental values through ideal mixing relation followed by Nomoto Relation in EDM + 1- butanol and DEM + 1- pentanol systems. It is observed that Nonoto's relation hold good in DEM + 1- Hexanol system followed by ideal mixing relation. There are higher variations in some intermediate concentration range suggesting the existence of strong tendency of association between component molecules as a result of hydrogen bonding[2].

Nomoto's theory proposes that the volume does not change upon mixing. Therefore, no interaction between the components of liquid mixtures has been taken into account. Similarly, the assumption for the formation of ideal mixing relation is that, the ratios of specific heats of ideal mixtures and the volumes are also equal. Again no molecular interactions are taken into account. But upon mixing, interactions between the molecules occur because of the presence of various types of forces such as dispersion forces, charge transfer, hydrogen bonding dipole-dipole and dipole-induced dipole interactions. Thus, the observed deviation of theoretical values of ve-

TABLE 1 : Experimental theoretical values of velocities with their percentage of deviations for the system Dem + 1- butanol at 303.15,308.15,313.15 and 318.15K

X_1	U_{EXP}	U_{NOM}	U_{IMP}	U_{VDV}	U_{JUN}	U_{RAO}	$\%U_N$	$\%U_{imp}$	$\%U_{VDV}$	$\%U_{JUN}$	$\%U_{RAO}$	U^2/U^2_{imx}
303.15K												
0.0000	1236.0	1236.0	1236.0	1236.0	1236.0	1236.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0578	1239.5	1237.5	1238.8	1237.0	1236.4	1250.8	-0.1583	-0.0599	-0.2036	-0.2491	0.9121	1.0041
0.1212	1242.9	1239.3	1241.7	1238.2	1237.0	1297.7	-0.2895	-0.0955	-0.3761	-0.4753	4.4118	1.0076
0.1913	1246.5	1241.3	1244.9	1239.8	1237.8	1405.8	-0.4136	-0.1295	-0.5358	-0.6974	12.7827	1.0108
0.2689	1250.1	1243.7	1248.3	1241.9	1239.0	1420.9	-0.5089	-0.1436	-0.6591	-0.8914	13.6594	1.0133
0.3556	1253.9	1246.6	1252.0	1244.5	1240.6	1517.7	-0.5834	-0.1518	-0.7516	-1.0608	21.0413	1.0152
0.4529	1258.0	1250.0	1256.0	1247.8	1243.0	1567.7	-0.6342	-0.1593	-0.8070	-1.1937	24.6184	1.0163
0.5629	1262.1	1254.3	1260.3	1252.2	1246.5	1585.2	-0.6215	-0.1391	-0.7823	-1.2335	25.6038	1.0158
0.6882	1266.4	1259.6	1265.1	1258.0	1252.0	1480.6	-0.5368	-0.1036	-0.6651	-1.1374	16.9118	1.0134
0.8324	1271.1	1266.6	1270.3	1265.6	1260.8	1404.0	-0.3570	-0.0642	-0.4303	-0.8096	10.4527	1.0087
1.0000	1276.0	1276.0	1276.0	1276.0	1276.0	1276.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	-0.0412	-0.0105	-0.0524	-0.0782	1.0993						
	$\chi 2$	0.2619	0.0167	0.4224	0.9552	310.8175						
308.15K												
0.0000	1217.0	1217.0	1217.0	1217.0	1217.0	1217.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0578	1220.9	1218.9	1220.4	1218.7	1217.8	1239.6	-0.1612	-0.0369	-0.1835	-0.2571	1.5349	1.0037
0.1212	1224.8	1221.1	1224.1	1220.6	1218.7	1282.8	-0.2983	-0.0534	-0.3394	-0.4945	4.7372	1.0068
0.1913	1229.2	1223.7	1228.1	1223.0	1220.0	1390.8	-0.4465	-0.0878	-0.5019	-0.7463	13.1495	1.0101
0.2689	1233.6	1226.7	1232.4	1225.9	1221.7	1408.9	-0.5578	-0.0970	-0.6221	-0.9620	14.2142	1.0126
0.3556	1238.4	1230.3	1237.0	1229.5	1224.0	1433.3	-0.6548	-0.1105	-0.7210	-1.1594	15.7401	1.0146
0.4529	1243.5	1234.6	1242.0	1233.9	1227.2	1436.6	-0.7152	-0.1167	-0.7756	-1.3070	15.5320	1.0157
0.5629	1248.6	1239.9	1247.5	1239.3	1231.8	1475.4	-0.6950	-0.0875	-0.7414	-1.3429	18.1610	1.0150
0.6882	1254.1	1246.6	1253.5	1246.3	1238.6	1478.4	-0.5956	-0.0503	-0.6209	-1.2322	17.8885	1.0125
0.8324	1260.3	1255.4	1260.0	1255.3	1249.3	1412.0	-0.3917	-0.0235	-0.3952	-0.8723	12.0370	1.0080
1.0000	1267.2	1267.2	1267.2	1267.2	1267.2	1267.2	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	-0.0454	-0.0066	-0.0493	-0.0846	0.9843						
	$\chi 2$	0.3178	0.0072	0.3728	1.1110	209.4672						
313.15K												
0.0000	1191.0	1191.0	1191.0	1191.0	1191.0	1191.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0578	1195.7	1193.4	1195.6	1193.6	1191.9	2200.0	-0.1891	-0.0120	-0.1741	-0.3141	83.9926	1.0035
0.1212	1200.5	1196.2	1200.4	1196.6	1193.2	2028.2	-0.3547	-0.0061	-0.3217	-0.6112	68.9471	1.0065
0.1913	1205.8	1199.5	1205.6	1200.1	1194.8	1838.2	-0.5228	-0.0130	-0.4688	-0.9158	52.4440	1.0094
0.2689	1211.5	1203.3	1211.2	1204.3	1196.9	1637.2	-0.6750	-0.0210	-0.5973	-1.2066	35.1366	1.0121
0.3556	1217.6	1207.9	1217.3	1209.1	1199.8	1480.5	-0.7980	-0.0266	-0.6947	-1.4643	21.5953	1.0140
0.4529	1224.2	1213.4	1223.8	1215.0	1203.8	1319.8	-0.8810	-0.0337	-0.7525	-1.6663	7.8128	1.0152
0.5629	1230.9	1220.3	1230.8	1222.1	1209.6	1180.5	-0.8643	-0.0050	-0.7158	-1.7297	-4.0948	1.0145
0.6882	1238.3	1229.0	1238.5	1230.9	1218.3	979.3	-0.7545	0.0161	-0.6016	-1.6126	-20.9173	1.0121
0.8324	1246.6	1240.4	1246.9	1241.9	1232.2	844.8	-0.4999	0.0204	-0.3803	-1.1562	-32.2313	1.0077
1.0000	1256.0	1256.0	1256.0	1256.0	1256.0	1256.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	-0.0558	-0.0008	-0.0473	-0.1083	0.9359						
	$\chi 2$	0.4737	0.0004	0.3398	1.7921	2145.4324						

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X_1	U_{EXP}	U_{NOM}	U_{IMP}	U_{VDV}	U_{JUN}	U_{RAO}	$\%U_N$	$\%U_{imp}$	$\%U_{VDV}$	$\%U_{JUN}$	$\%U_{RAO}$	U^2/U^2_{imx}
318.15K												
0.0000	1177.0	1177.0	1177.0	1177.0	1177.0	1177.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0578	1181.6	1179.5	1181.7	1179.8	1177.9	2236.2	-0.1783	0.0112	-0.1559	-0.3122	89.2486	1.0031
0.1212	1186.5	1182.4	1186.8	1182.9	1179.1	2044.6	-0.3489	0.0239	-0.3012	-0.6237	72.3261	1.0061
0.1913	1191.8	1185.7	1192.2	1186.6	1180.7	1857.2	-0.5125	0.0325	-0.4367	-0.9339	55.8318	1.0088
0.2689	1197.7	1189.6	1198.0	1190.9	1182.8	1654.7	-0.6753	0.0236	-0.5690	-1.2457	38.1569	1.0115
0.3556	1204.0	1194.3	1204.2	1195.9	1185.7	1487.3	-0.8064	0.0177	-0.6688	-1.5221	23.5332	1.0135
0.4529	1210.8	1200.0	1210.9	1202.0	1189.7	1330.2	-0.8942	0.0106	-0.7271	-1.7391	9.8583	1.0147
0.5629	1217.8	1207.0	1218.2	1209.3	1195.7	1171.3	-0.8854	0.0320	-0.6967	-1.8183	-3.8195	1.0141
0.6882	1225.5	1216.0	1226.1	1218.3	1204.6	984.2	-0.7765	0.0461	-0.5864	-1.7040	-19.6885	1.0118
0.8324	1234.1	1227.8	1234.6	1229.6	1219.0	847.0	-0.5120	0.0435	-0.3663	-1.2242	-31.3630	1.0074
1.0000	1244.0	1244.0	1244.0	1244.0	1244.0	1244.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	-0.0563	0.0024	-0.0453	-0.1129	1.0642						
	χ2	0.4809	0.0009	0.3108	1.9361	2356.8518						

TABLE 2: Experimental theoretical values of velocities with their percentage of deviations for the system Dem + 1- pentanol at 303.15,308.15,313.15 and 318.15K

X_1	U_{EXP}	U_{NOM}	U_{IMP}	U_{VDV}	U_{JUN}	U_{RAO}	$\%U_N$	$\%U_{imp}$	$\%U_{VDV}$	$\%U_{JUN}$	$\%U_{RAO}$	U^2/U^2_{imx}
303.15K												
0.0000	1259.0	1259.0	1259.0	1259.0	1259.0	1259.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0732	1260.9	1259.8	1260.5	1258.3	1258.6	1262.9	-0.0842	-0.0332	-0.2083	-0.1798	0.1606	1.0042
0.1510	1263.0	1260.8	1262.0	1257.8	1258.4	1299.3	-0.1761	-0.0787	-0.4085	-0.3667	2.8702	1.0082
0.2336	1264.9	1261.8	1263.6	1257.8	1258.3	1396.3	-0.2424	-0.1048	-0.5646	-0.5251	10.3915	1.0114
0.3217	1266.8	1263.0	1265.2	1258.1	1258.4	1401.2	-0.2973	-0.1271	-0.6866	-0.6654	10.6131	1.0139
0.4157	1268.6	1264.4	1266.9	1259.0	1258.8	1488.0	-0.3303	-0.1375	-0.7600	-0.7716	17.2943	1.0154
0.5162	1270.2	1266.0	1268.6	1260.4	1259.7	1530.7	-0.3306	-0.1282	-0.7684	-0.8238	20.5075	1.0155
0.6240	1271.7	1267.9	1270.3	1262.7	1261.4	1545.5	-0.3018	-0.1068	-0.7090	-0.8109	21.5285	1.0143
0.7399	1273.2	1270.1	1272.2	1265.9	1264.1	1446.6	-0.2458	-0.0811	-0.5761	-0.7108	13.6223	1.0116
0.8649	1274.6	1272.7	1274.1	1270.2	1268.7	1382.3	-0.1466	-0.0429	-0.3446	-0.4665	8.4495	1.0069
1.0000	1276.0	1276.0	1276.0	1276.0	1276.0	1276.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	-0.0216	-0.0084	-0.0506	-0.0536	0.9122						
	χ2	0.0732	0.0114	0.3962	0.4494	211.9999						
308.15K												
0.0000	1244.8	1244.8	1244.8	1244.8	1244.8	1244.8	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0732	1246.9	1245.9	1246.7	1244.6	1244.7	1256.8	-0.0797	-0.0124	-0.1872	-0.1764	0.7980	1.0038
0.1510	1249.3	1247.1	1248.7	1244.6	1244.7	1289.6	-0.1725	-0.0442	-0.3736	-0.3653	3.2265	1.0075
0.2336	1251.6	1248.5	1250.8	1245.1	1245.0	1387.0	-0.2445	-0.0630	-0.5223	-0.5303	10.8200	1.0105
0.3217	1254.0	1250.1	1252.9	1245.9	1245.5	1394.9	-0.3091	-0.0847	-0.6437	-0.6814	11.2388	1.0130
0.4157	1256.3	1251.9	1255.1	1247.3	1246.3	1410.4	-0.3472	-0.0931	-0.7150	-0.7935	12.2695	1.0145
0.5162	1258.4	1254.0	1257.4	1249.3	1247.8	1407.5	-0.3468	-0.0801	-0.7198	-0.8456	11.8468	1.0146
0.6240	1260.5	1256.5	1259.7	1252.1	1250.0	1442.6	-0.3182	-0.0614	-0.6631	-0.8332	14.4449	1.0134
0.7399	1262.7	1259.4	1262.1	1255.9	1253.5	1447.9	-0.2615	-0.0447	-0.5393	-0.7320	14.6642	1.0109
0.8649	1264.8	1262.9	1264.6	1260.8	1258.8	1392.1	-0.1502	-0.0137	-0.3152	-0.4740	10.0644	1.0063
1.0000	1267.2	1267.2	1267.2	1267.2	1267.2	1267.2	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	-0.0224	-0.0050	-0.0471	-0.0547	0.7986						
	χ2	0.0785	0.0043	0.3420	0.4666	134.7112						

X_1	U_{EXP}	U_{NOM}	U_{IMP}	U_{VDV}	U_{JUN}	U_{RAO}	$\%U_N$	$\%U_{imp}$	$\%U_{VDV}$	$\%U_{JUN}$	$\%U_{RAO}$	U^2/U^2_{imx}
313.15K												
0.0000	1221.0	1221.0	1221.0	1221.0	1221.0	1221.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0732	1224.0	1222.7	1224.1	1221.9	1221.1	2233.8	-0.1072	0.0082	-0.1738	-0.2344	82.5040	1.0035
0.1510	1227.2	1224.6	1227.3	1223.1	1221.5	2040.3	-0.2133	0.0065	-0.3360	-0.4677	66.2589	1.0068
0.2336	1230.5	1226.7	1230.5	1224.7	1222.1	1833.0	-0.3070	0.0035	-0.4735	-0.6855	48.9606	1.0095
0.3217	1234.1	1229.2	1233.9	1226.7	1223.1	1619.6	-0.4002	-0.0169	-0.5967	-0.8950	31.2347	1.0120
0.4157	1237.5	1232.0	1237.3	1229.4	1224.6	1454.8	-0.4474	-0.0137	-0.6580	-1.0433	17.5581	1.0133
0.5162	1240.9	1235.2	1240.9	1232.7	1226.9	1290.5	-0.4579	-0.0031	-0.6648	-1.1275	3.9996	1.0134
0.6240	1244.4	1239.0	1244.5	1236.8	1230.4	1151.7	-0.4304	0.0072	-0.6142	-1.1265	-7.4491	1.0124
0.7399	1248.0	1243.6	1248.2	1241.9	1235.6	957.0	-0.3519	0.0176	-0.4925	-0.9934	-23.3190	1.0099
0.8649	1251.8	1249.1	1252.1	1248.2	1243.6	831.6	-0.2122	0.0204	-0.2900	-0.6585	-33.5643	1.0058
1.0000	1256.0	1256.0	1256.0	1256.0	1256.0	1256.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	-0.0294	0.0003	-0.0432	-0.0730	0.7153						
	χ2	0.1333	0.0002	0.2852	0.8181	2043.2319						
318.15K												
0.0000	1204.0	1204.0	1204.0	1204.0	1204.0	1204.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0732	1207.3	1205.9	1207.6	1205.3	1204.2	2265.3	-0.1150	0.0223	-0.1643	-0.2550	87.6312	1.0033
0.1510	1210.8	1208.1	1211.2	1207.0	1204.7	2051.8	-0.2263	0.0350	-0.3160	-0.5066	69.4602	1.0063
0.2336	1214.5	1210.5	1215.0	1209.0	1205.4	1847.2	-0.3303	0.0386	-0.4498	-0.7477	52.0982	1.0091
0.3217	1218.4	1213.3	1218.8	1211.6	1206.6	1632.7	-0.4219	0.0334	-0.5598	-0.9684	34.0008	1.0113
0.4157	1222.3	1216.4	1222.7	1214.7	1208.4	1457.7	-0.4788	0.0362	-0.6225	-1.1380	19.2582	1.0126
0.5162	1226.2	1220.2	1226.8	1218.5	1211.1	1297.4	-0.4927	0.0470	-0.6288	-1.2351	5.8068	1.0127
0.6240	1230.2	1224.5	1230.9	1223.1	1215.0	1140.2	-0.4611	0.0582	-0.5760	-1.2348	-7.3198	1.0116
0.7399	1234.5	1229.8	1235.2	1228.7	1220.9	960.0	-0.3847	0.0537	-0.4663	-1.1000	-22.2320	1.0094
0.8649	1239.0	1236.1	1239.5	1235.6	1229.9	832.9	-0.2337	0.0422	-0.2739	-0.7336	-32.7756	1.0055
1.0000	1244.0	1244.0	1244.0	1244.0	1244.0	1244.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	-0.0316	0.0037	-0.0408	-0.0800	0.8372						
	χ2	0.1517	0.0020	0.2509	0.9701	2231.9593						

TABLE 3: Experimental theoretical values of velocities with their percentage of deviations for the system Dem + 1- hexanol at 303.15,308.15,313.15 and 318.15K

X_1	U_{EXP}	U_{NOM}	U_{IMP}	U_{VDV}	U_{JUN}	U_{RAO}	$\%U_N$	$\%U_{imp}$	$\%U_{VDV}$	$\%U_{JUN}$	$\%U_{RAO}$	U^2/U^2_{imx}
303.15K												
0.0000	1288.5	1288.5	1288.5	1288.5	1288.5	1288.5	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0834	1287.8	1287.8	1287.3	1284.6	1286.7	1283.7	-0.0007	-0.0418	-0.2460	-0.0874	-0.3165	1.0049
0.1700	1287.1	1287.0	1286.0	1281.2	1284.8	1312.2	-0.0070	-0.0838	-0.4592	-0.1767	1.9538	1.0092
0.2598	1286.4	1286.1	1284.8	1278.2	1283.0	1402.1	-0.0198	-0.1260	-0.6362	-0.2662	8.9977	1.0128
0.3532	1285.6	1285.2	1283.5	1275.8	1281.2	1400.0	-0.0323	-0.1608	-0.7652	-0.3458	8.8953	1.0155
0.4503	1284.6	1284.1	1282.3	1273.9	1279.4	1480.5	-0.0382	-0.1803	-0.8339	-0.4040	15.2503	1.0169
0.5513	1283.2	1282.9	1281.0	1272.7	1277.8	1518.5	-0.0236	-0.1689	-0.8217	-0.4199	18.3385	1.0166
0.6565	1281.4	1281.5	1279.8	1272.1	1276.5	1531.0	0.0095	-0.1265	-0.7219	-0.3853	19.4797	1.0146
0.7662	1279.6	1279.9	1278.5	1272.5	1275.5	1433.8	0.0272	-0.0843	-0.5579	-0.3185	12.0507	1.0113
0.8806	1277.8	1278.1	1277.3	1273.7	1275.2	1374.0	0.0257	-0.0421	-0.3209	-0.2003	7.5308	1.0064
1.0000	1276.0	1276.0	1276.0	1276.0	1276.0	1276.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	-0.0006	-0.0102	-0.0540	-0.0261	0.8081						
	χ2	0.0006	0.0175	0.4580	0.1102	168.5742						

X_1	U_{EXP}	U_{NOM}	U_{IMP}	U_{VDV}	U_{JUN}	U_{RAO}	$\%U_N$	$\%U_{imp}$	$\%U_{VDV}$	$\%U_{JUN}$	$\%U_{RAO}$	U^2/U^2_{imx}
308.15K												
0.0000	1279.2	1279.2	1279.2	1279.2	1279.2	1279.2	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0834	1278.4	1278.5	1278.0	1275.4	1277.4	1282.6	0.0091	-0.0301	-0.2344	-0.0746	0.3278	1.0047
0.1700	1277.7	1277.8	1276.8	1272.0	1275.7	1307.4	0.0051	-0.0683	-0.4439	-0.1587	2.3244	1.0089
0.2598	1277.0	1276.9	1275.6	1269.1	1273.9	1397.7	-0.0053	-0.1068	-0.6172	-0.2430	9.4519	1.0125
0.3532	1276.2	1276.0	1274.4	1266.7	1272.2	1398.2	-0.0150	-0.1378	-0.7425	-0.3173	9.5590	1.0150
0.4503	1275.2	1275.0	1273.2	1264.9	1270.5	1407.5	-0.0177	-0.1534	-0.8076	-0.3703	10.3717	1.0163
0.5513	1273.9	1273.8	1272.0	1263.7	1268.9	1399.9	-0.0070	-0.1459	-0.7991	-0.3888	9.8871	1.0162
0.6565	1272.2	1272.5	1270.8	1263.3	1267.7	1432.1	0.0228	-0.1072	-0.7029	-0.3572	12.5652	1.0142
0.7662	1270.5	1271.0	1269.6	1263.6	1266.8	1437.2	0.0378	-0.0686	-0.5426	-0.2946	13.1208	1.0109
0.8806	1268.8	1269.2	1268.4	1264.9	1266.5	1384.9	0.0344	-0.0303	-0.3092	-0.1826	9.1525	1.0062
1.0000	1267.2	1267.2	1267.2	1267.2	1267.2	1267.2	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	0.0006	-0.0085	-0.0523	-0.0239	0.6950						
	χ2	0.0005	0.0125	0.4281	0.0926	102.5313						
X_1	U_{EXP}	U_{NOM}	U_{IMP}	U_{VDV}	U_{JUN}	U_{RAO}	$\%U_N$	$\%U_{imp}$	$\%U_{VDV}$	$\%U_{JUN}$	$\%U_{RAO}$	U^2/U^2_{imx}
313.15K												
0.0000	1275.2	1275.2	1275.2	1275.2	1275.2	1275.2	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0834	1273.8	1274.1	1273.3	1270.6	1272.9	2313.2	0.0257	-0.0418	-0.2474	-0.0730	81.5960	1.0050
0.1700	1272.3	1272.9	1271.3	1266.5	1270.5	2095.6	0.0505	-0.0756	-0.4535	-0.1429	64.7084	1.0091
0.2598	1270.8	1271.6	1269.4	1262.9	1268.1	1868.2	0.0654	-0.1093	-0.6226	-0.2162	47.0106	1.0126
0.3532	1269.3	1270.2	1267.5	1259.8	1265.6	1639.2	0.0683	-0.1428	-0.7508	-0.2905	29.1405	1.0152
0.4503	1267.6	1268.5	1265.6	1257.2	1263.2	1463.4	0.0730	-0.1605	-0.8178	-0.3467	15.4445	1.0166
0.5513	1265.5	1266.7	1263.6	1255.3	1260.9	1291.6	0.0925	-0.1464	-0.8027	-0.3633	2.0658	1.0162
0.6565	1263.2	1264.6	1261.7	1254.2	1258.8	1148.6	0.1076	-0.1163	-0.7146	-0.3477	-9.0742	1.0144
0.7662	1260.8	1262.1	1259.8	1253.8	1257.1	952.7	0.1056	-0.0779	-0.5538	-0.2943	-24.4338	1.0112
0.8806	1258.4	1259.3	1257.9	1254.4	1256.0	828.5	0.0725	-0.0391	-0.3191	-0.1898	-34.1612	1.0064
1.0000	1256.0	1256.0	1256.0	1256.0	1256.0	1256.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	0.0066	-0.0091	-0.0532	-0.0227	0.5996						
	χ2	0.0068	0.0137	0.4371	0.0826	2032.7528						
318.15K												
0.0000	1258.4	1258.4	1258.4	1258.4	1258.4	1258.4	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
0.0834	1257.3	1257.6	1256.9	1254.4	1256.2	2347.0	0.0240	-0.0286	-0.2314	-0.0854	86.6714	1.0046
0.1700	1256.1	1256.7	1255.5	1250.8	1254.0	2108.2	0.0494	-0.0490	-0.4218	-0.1654	67.8339	1.0085
0.2598	1255.0	1255.7	1254.0	1247.7	1251.8	1883.1	0.0592	-0.0770	-0.5837	-0.2539	50.0482	1.0118
0.3532	1253.9	1254.7	1252.6	1245.1	1249.6	1652.5	0.0599	-0.1047	-0.7052	-0.3398	31.7863	1.0143
0.4503	1252.6	1253.4	1251.1	1243.0	1247.6	1466.1	0.0658	-0.1161	-0.7659	-0.4025	17.0464	1.0155
0.5513	1251.0	1252.0	1249.7	1241.6	1245.7	1298.2	0.0828	-0.1033	-0.7524	-0.4270	3.7747	1.0152
0.6565	1249.3	1250.5	1248.3	1240.9	1244.1	1136.7	0.0922	-0.0821	-0.6741	-0.4182	-9.0114	1.0136
0.7662	1247.6	1248.6	1246.8	1241.0	1243.0	955.5	0.0823	-0.0605	-0.5315	-0.3672	-23.4121	1.0107
0.8806	1245.8	1246.5	1245.4	1242.0	1242.8	829.6	0.0565	-0.0305	-0.3077	-0.2396	-33.4076	1.0062
1.0000	1244.0	1244.0	1244.0	1244.0	1244.0	1244.0	0.0000	0.0000	0.0000	0.0000	0.0000	1.0000
	σ	0.0057	-0.0065	-0.0500	-0.0271	0.7188						
	χ2	0.0050	0.0070	0.3823	0.1159	2219.2578						

locity from the experimental values shows that the molecular interactions are taking place between the

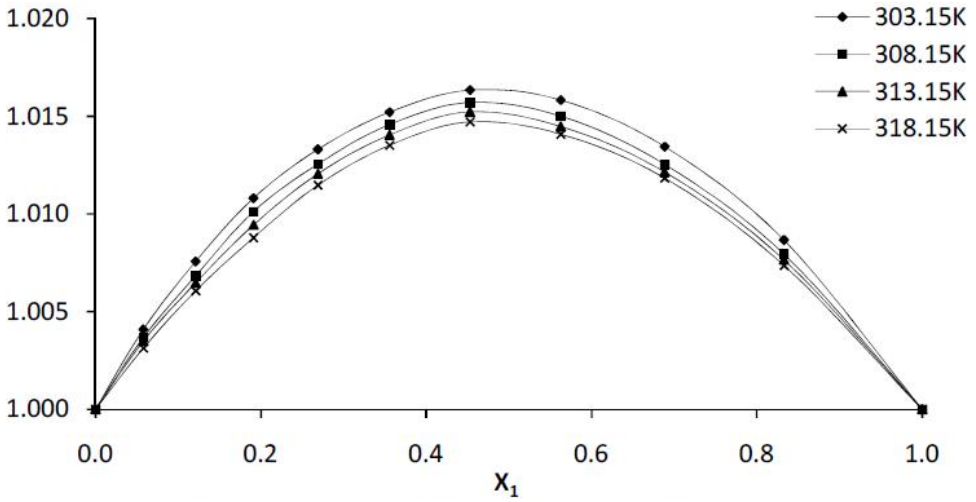

Figure 1 : Variation of U2 exp/U2 imx with the mole fraction of DEM for the system DEM + 1- butanol

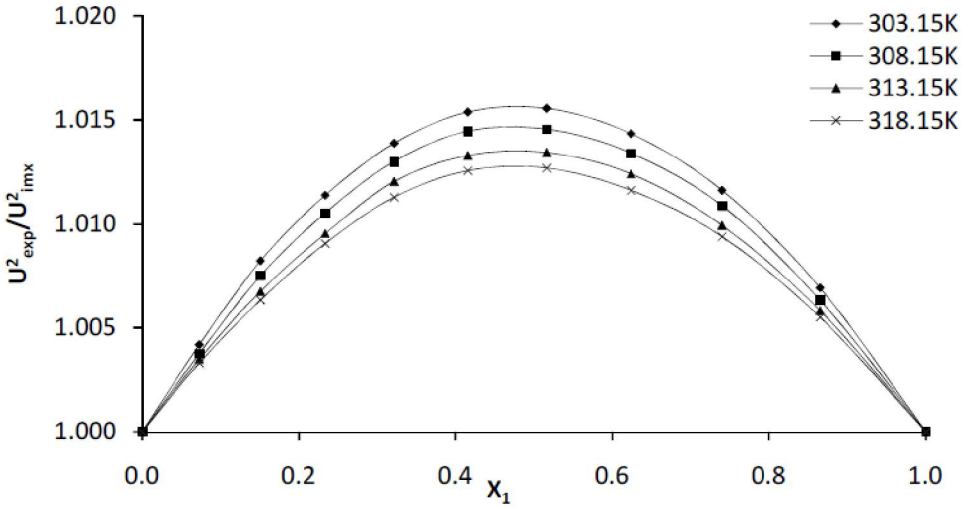

Figure 2 : Variation of U2 exp/U2imx with the mole fraction of DEM for DEM + 1- Pentanol system

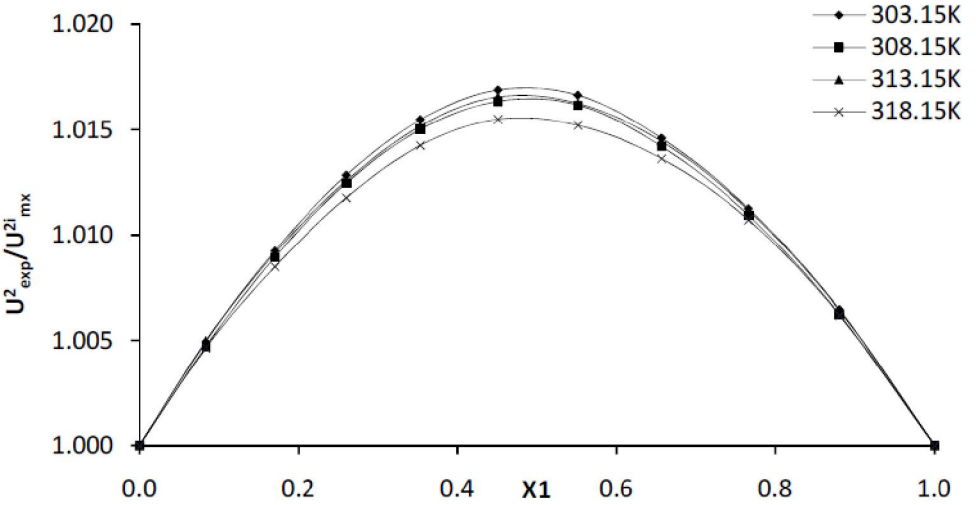

Figure 3 : Variation of U2 exp/U2 imx with the mole fraction of DEM for the system DEM + 1- hexanol

unlike molecules[1].

The magnitude of the chi-square value finally determines the overall validity of the theory[19]. The chi square values along with standard deviation are

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given in TABLES 1,2 and 3. Figures 1,2 and 3 give the variation of (U^2/U^2_{imx}) for the systems DEM + 1-butanol, 1-pentanol and 1-Hexnol respectively at temperatures 303.15K,308.15K,313.15K and 318.15K against the mole fraction of DEM.

On the whole, all the theoretical models fairly predicted ultrasonic velocities, are reasonably close to the experimental values for and the three binary mixtures reported in this work, thus showing the validity of studied theoretical models for binary mixtures. The predictive abilities of various ultrasonic theories discussed above, depend upon the strength interaction prevailing in a system. In general the predictive ability of various ultrasonic theories depends upon the strength of interactions that exist in a binary system. In case strong interactions exist between the molecules of the mixtures there is much deviation in theoretical prediction of velocity than the molecules of the mixture where less interaction are present, and the average absolute percentage relative deviation is small in systems where the interactions are less or nil.

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