Research Article

Theoretical Evaluation of Ultrasonic Velocity in 1,4 Dioxane with 1-Butnaol at Temperatures Range 298.15-318.15K

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ABSTRACT

Theoretical values of Ultrasonic Velocity in binary liquid mixture of 1,4 Dioxane with 1-Butanol for different proportions have been evaluated using Nomoto's, Ideal Mixture Relation, Impedance Relation. Further, the experimental Ultrasonic velocities of the binary mixture are compared with Ultrasonic velocity, in the temperatures range 298.15-318.15 K.

Keywords: Ultrasonic velocity, 1-4 Dioxane, 1-Butanol, Nomoto's, Ideal Mixture Relation.

1. INTRODUCTION

In the field of Ultrasonics, it became important day by day to study theoretical and experimental investigation with much effort. Hence it is decided to evaluate the theoretical ultrasonic velocities of the selected binary mixture when it is exposed to ultrasonic waves. The ultrasonic velocity measurements have been widely used to study the physical and chemical behavior of liquid mixtures. In recent years a good amount of work has been done to correlate the experimental ultrasonic velocities with those computed standard theoretical relations namely, Nomoto's, impedance, and vandal[1], Further, the study of thermodynamic behavior for the mixtures of branched or cyclic ethers such as 1,4-dioxane, 1,3-dioxolane, 1,3,5-trioxane etc., may be used as fuel additives, commercially used in polymerization, other chemical reactions in the cleaning of polymer surfaces and electronic materials, in near future, with different organic liquids are studied by many of the researchers[2-8].

In the present paper, the theoretical approaches for liquids namely Nomoto relation (u^{NOM}) Impedance dependence relation, ,Vandael Vangeal ideal mixing relation (u^{VAN}) and impedance applied to the binary under investigation at all five temperatures reflect the behaviour of the system by measuring the deviation of the theoretical values of sound speeds from experi-mental ones.

2. EXPERIMENTAL DETAILS

1,4 dioxane, butan-1-ol used in this investigation were the same as used in our earlier works[1,2]. 1,4-Dioxane with mass fraction purities >0.998 were purchased from Aldrich Chemical Co. the chemicals were kept in airtight stopped glass bottles. Mole fractions of these samples were determined by measuring the mass of each component with a precision balance (Sartorius, model CP 225D, +/-0.01mg). The uncertainty of the compostion on a mole fracion basis was 0.0001. The ultrasonic velocity, densitites of pure components and binary mixtures at different temperatures were obtained with a vibrating-tube densimeter (Anton Paar DSA 5000M). The uncertainty of density is +/- 0.000005 $g*cm^{-3}$. The densimeter was calibrated with ultrapure water, and densitites have been listed in Table 1, compared with literature.

3. THEORETICAL ASPECT

The different theoretical considerations for the empirical formula for sound speed in binary liquid mixtures given by Nomoto[9] can be written as:

Nomoto's relation:

$U_N = [(x_1R_1+x_2R_2) /(x_1V_1+x_2V_2)]^3$ (1)

where x, *R* and *V* represents mole fraction, molar sound speed and molar volume, respectively.

Impedance dependent relation:

$U_{Imp} = \Sigma x_iZ_i / \Sigma x_i\rho_i$ (2)

Where X_i is mole fraction, Z_i is acoustic impedance, ρ_i density of the i^{th} component

Van Dael ideal mixing relation[10]:

$Uvdv = [(x_1/M_1U^2{}_1 + /M_2U^2{}_2)(x_1M_1+x_2M_2)]^{-1/2}$ (3)

where x_1 and x_2 are mole fractions of 1,4-dioxane and butan-1-ol respectively, at the temperature range. (298.15K, 303.15K, 308.15K, 313.15K, and 318.15K)

4. RESULTS AND DISCUSSION

Comparison of theoretical values of ultrasonic velocities with those obtained experimentally in the present binary liquid mixture is expected to reveal the nature of interaction between the component molecules in the mixture. Table-1 shows observed and literature values of ultrasonic velocity, density for 1,4 Dioxane and 1-butanol.

Table 1: Observed and literature values of ultrasonic velocity, density for 1, 4 Dioxane and 1-butanol

Compound	T	Ultrasonic velocity (u)		Density (ρ)	
		Observed	Literature	Observed	Literature
1,4-dioxane	298.15 K	1344.3	1344.8[11,12]	1026.8	1027.9[11,13]
	303.15 K			1021.2	1022.5[14,15]
1-butanol	298.15 K	1240.6	1240[16]	806.6	806.3[16]
	303.15 K	1223.7	1228.8[17]	802.7	802[18,19]

using the equations[20-21], theoretical values of ultrasonic velocities calculated along with the experimental values for the liquid mixture at temperatures (298.15K,303.15K, 308.15K, 313.15K, and 318.15K) are given in Tables 2. It is observed that the theoretical values of ultrasonic velocity calculated by using various theories shows deviation from experimental values. The limitations and approximation of these theories are responsible for the deviations in between theoretical and experimental values.

In the present study, the deviations of experimental and theoretical values in respective theories are as follows.

According to Nomoto's theory, it is well understood that the volume does not change on mixing of the liquids but there exists various types forces, ex: charge transfer , dipole-dipole, dipole-induced dipole, dispersive forces, hydrogen bond etc., interactions exists between the molecules of the two liquids, are responsible for the deviations of experimental values from theoretical values. In the case of Van Dael Ideal mixture relation the deviation might be due to the compressibility of the component liquids. Whereas the values calculated from impedance relation shows non-additivity of acoustic impedance in the liquid mixture.

Table 2: Application of various theoretical approaches for 1, 4 Dioxane and 1-butanol system at 298.15 K to 323.15 K

Mole fraction of 1,4 D0	U_{EXP} ms^{-1}	U_N ms^{-}	U_{IMP} ms^{-1}	U_{VDV} ms^{-1}	% deviations		
					U_N ms^{-1}	U_{IMP} ms^{-1}	U_{VDV} ms^{-1}
T=298.15 K							
0.0000	1240.6	1240.6	1240.6	1160.1	0.00	0.00	6.49
0.1149	1247.5	1248.6	1255.3	1178.6	-0.09	-0.62	5.52
0.2123	1254.6	1255.9	1267.1	1194.8	-0.10	-0.99	4.77
0.3037	1262.3	1263.3	1277.6	1210.4	-0.08	-1.22	4.11
0.4068	1272.0	1272.3	1288.9	1228.5	-0.03	-1.33	3.42
0.5112	1282.5	1282.3	1299.8	1247.4	0.02	-1.35	2.74
0.6297	1296.0	1294.8	1311.5	1269.5	0.10	-1.20	2.04
0.7066	1305.9	1303.6	1318.8	1284.4	0.18	-0.99	1.65
0.7993	1317.2	1315.2	1327.2	1302.7	0.15	-0.76	1.10
0.9065	1331.6	1330.0	1336.5	1324.6	0.12	-0.37	0.53
1.0000	1344.3	1344.3	1344.3	1344.3	0.00	0.00	0.00
T=303.15 K							
0.0000	1223.7	1223.7	1223.7	1152.1	0.00	0.00	5.85
0.1149	1229.4	1231.3	1237.7	1169.4	-0.16	-0.67	4.88
0.2123	1237.0	1238.3	1248.9	1184.4	-0.10	-0.96	4.25
0.3037	1244.2	1245.3	1258.9	1198.9	-0.09	-1.18	3.65
0.4068	1253.5	1253.9	1269.6	1215.6	-0.03	-1.29	3.02
0.5112	1263.4	1263.4	1280.0	1233.1	0.00	-1.32	2.40
0.6297	1275.8	1275.3	1291.1	1253.6	0.04	-1.20	1.74
0.7066	1284.9	1283.7	1298.0	1267.2	0.10	-1.02	1.38

0.7993	1296.6	1294.7	1306.1	1284.1	0.15	-0.73	0.96
0.9065	1310.3	1308.7	1314.9	1304.2	0.12	-0.35	0.47
1.0000	1322.3	1322.3	1322.3	1322.3	0.00	0.00	0.00
T=308.15 K							
0.0000	1206.9	1206.9	1206.9	1136.3	0.00	0.00	5.85
0.1149	1212.2	1214.1	1220.1	1153.0	-0.16	-0.66	4.89
0.2123	1219.4	1220.7	1230.8	1167.5	-0.11	-0.93	4.26
0.3037	1226.2	1227.4	1240.3	1181.4	-0.10	-1.15	3.65
0.4068	1235.1	1235.6	1250.5	1197.6	-0.04	-1.25	3.03
0.5112	1245.2	1244.6	1260.3	1214.5	0.05	-1.22	2.46
0.6297	1257.6	1255.9	1270.9	1234.2	0.14	-1.06	1.86
0.7066	1266.2	1263.8	1277.4	1247.4	0.19	-0.89	1.49
0.7993	1276.1	1274.3	1285.1	1263.7	0.14	-0.71	0.97
0.9065	1289.2	1287.6	1293.5	1283.1	0.12	-0.34	0.47
1.0000	1300.5	1300.5	1300.5	1300.5	0.00	0.00	0.00
T=308.15 K							
0.0000	1190.1	1190.1	1190.1	1120.6	0.00	0.00	5.85
0.1149	1195.1	1197.0	1202.7	1136.6	-0.16	-0.64	4.89
0.2123	1201.8	1203.2	1212.7	1150.6	-0.12	-0.91	4.26
0.3037	1208.3	1209.5	1221.7	1164.1	-0.11	-1.11	3.66
0.4068	1216.6	1217.3	1231.3	1179.6	-0.05	-1.21	3.04
0.5112	1226.2	1225.8	1240.6	1195.9	0.04	-1.17	2.48
0.6297	1236.8	1236.4	1250.6	1214.9	0.04	-1.11	1.78
0.7066	1245.0	1243.9	1256.8	1227.5	0.08	-0.95	1.40
0.7993	1255.5	1253.8	1264.0	1243.2	0.14	-0.67	0.98
0.9065	1268.1	1266.4	1271.9	1261.8	0.14	-0.30	0.50
1.0000	1278.6	1278.6	1278.6	1278.6	0.00	0.00	0.00
T=318.15 K							
0.0000	1173.5	1173.5	1173.5	1104.9	0.00	0.00	5.85
0.1149	1178.0	1180.0	1185.3	1120.4	-0.16	-0.62	4.89
0.2123	1184.4	1185.9	1194.8	1133.9	-0.13	-0.89	4.26
0.3037	1190.4	1191.9	1203.4	1146.9	-0.13	-1.09	3.65
0.4068	1198.3	1199.3	1212.5	1161.9	-0.08	-1.19	3.03
0.5112	1206.9	1207.3	1221.3	1177.6	-0.03	-1.19	2.43
0.6297	1217.0	1217.4	1230.8	1195.9	-0.03	-1.13	1.73
0.7066	1225.0	1224.6	1236.7	1208.2	0.04	-0.95	1.37
0.7993	1235.3	1233.9	1243.5	1223.2	0.11	-0.67	0.97
0.9065	1247.1	1245.8	1251.0	1241.2	0.11	-0.31	0.48
1.0000	1257.3	1257.3	1257.3	1257.3	0.00	0.00	0.00

5. CONCLUSION

Theoretical evaluations of ultrasonic velocities in the binary liquid mixture by three different theories are determined, and compared the results with the experimentally obtained values. At the end, it is observed that, out of all the theories Nomoto's theory gives best results followed by Impedance dependence relation in the mixture studied.

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