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ORIGINAL ARTICLE

THEORETICAL EVALUATION OF ULTRASONIC VELOCITIES IN THE TERNARY LIQUID MIXTURES OF METHYL ISOBUTYL KETONE +BENZENE + ALKANOLS

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ABSTRACT

A comparison of ultrasonic velocity evaluated from Nomoto's relation, Van Deal-Vangeel ideal mixing relation, Impedance dependence relation, Rao's specific velocity and Junjie method with that of experimental values have been made in the ternary liquid mixtures of methyl isobutyl ketone with benzene and 1-alkanols. The relative applicability of these theories to the present systems has been checked and discussed.

Keywords: Ultrasonic Velocity, Methyl Isobutyl Ketone, Theoretical Evaluation

1.INTRODUCTION

Ultrasonic velocity in liquid mixtures have been calculated and compared with experimental values using various theories(Nomoto,1958; Van and Vangael,1955; Ernst et al., 1979; Jacobson,1952; Junjie,1984; Schaaffs,1963; Baluja andParasania,1995;GokhaleandBhagavat,1989; Kudriavtsev, 1956).This comparison is expected to reveal the nature of interaction between component molecules in the mixtures. It is also useful in defining a comprehensive theoretical model for a specific liquid mixture. In the present investigation, Methyl Isobutyl Ketone and Benzene is mixed with 1-Alkanols like 1-Propanol and 1- Butanol at different mole fractions to study the extent of interactions between dissimilar molecules.

2.THEORY

The following relations/ theories are used for the prediction of ultrasonic velocity in the binary liquid mixtures and is extended to ternary mixtures.

Nomoto's relation(NR)

Nomoto(1958) established on empirical formula for ultrasonic velocity (U) in binary liquid mixtures on the assumption of linear dependence of the molar sound velocity (R) on concentration in mole fraction (X_1 and X_2) and the addition of molar volume. The linearity of molar sound velocity can be expressed as

$R = X_1R_1 + X_2R_2$ ------- (1)

The molar sound velocity is related to molecular weight (M) and density (ρ) by

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

Where the molar volume V obeys the additively

$V = X_1U_1 + X_2U_2$ ----- (3)

Extending the same for ternary liquid mixtures the ultrasonic velocity is

$U_{NR} = [\frac{X_1R_1 + X_2R_2 + X_3R_3}{X_1V_1 + X_2V_2 + X_3V_3}]^3$ -------- (4)

Ideal mixture relation (IMR)

Van and Vangeel (1955) suggested the following relation for sound velocity

$$\frac{1}{(X_1M_1+X_2M_2+X_3M_3)Uim^2} = \frac{X_1}{X_1U_1^2} + \frac{X_2}{X_2U_2^2} + \frac{X_3}{X_3U_3^2} \text{ --(5)}$$

Where M is the molecular weight and X is the molar concentration

$$U_{IMR} = [\frac{X_1}{X_1U_1^2} + \frac{X_2}{X_2U_2^2} + \frac{X_3}{X_3U_3^2}]^{-1/2}[\frac{1}{X_1M_1+X_2M_2+X_3M_3}]^{1/2} \text{ -----(6)}$$

The degree of the molecular interaction parameter α can be computed from the equation

$\alpha = (U^2_{expt}/U^2_{IMR}) - 1$ ----------(7)

Junjie's method (JM)

Junjie(1984) has proposed equation for the evaluation of velocity of sound in a given liquid mixture, and is represented by

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$$U_j = \left[\frac{X_1M_1}{\rho_1} + \frac{X_2M_2}{\rho_2} + \frac{X_3M_3}{\rho_3}\right]\left[\frac{1}{X_1M_1+X_2M_2+X_3M_3}\right]^{1/2}\left[\frac{X_1M_1}{\rho_1U_1^2} + \frac{X_2M_2}{\rho_2U_2^2} + \frac{X_3M_3}{\rho_3U_3^2}\right]^{-1/2} \quad \text{----------8}$$

Where M_1, M_2 are molecular weights of constituent components. X_1 and X_2 are their mole fraction. ρ_1, ρ_2 , ρ_3 are their densities.

Impedance Relation (IR)

Impedance (Baluja and Parasania, 1995) is the product of ultrasonic velocity (U) and the density (P) of a liquid mixture. Hence the impedance relation predicts the ultrasonic Velocity of the given mixture by simply using the values of impedance (Z) and the density(P) values Impedance relation is given as

$$U_{IR} = \frac{\Sigma\ X_iZ_i}{\Sigma\ X_i\rho_i} \quad \text{---------(9)}$$

X_i – mole fraction, ρ_i is the density of the mixture and Z_i the acoustic impedance.

Rao's specific Velocity method Relation(U_R)

Rao's (Gokhale and Bhagavat, 1989) specific Velocity is given

$$U_R = [\ \Sigma\ X_iR_i\rho_i\ ]^3 \quad \text{----(10)}$$

Where x_i is the mole fraction, ρ_i is the density of the mixture. R_i is Rao's specific constant.

$R_i = \frac{M_i}{\rho_i U_i^{\frac{1}{3}}}$ Where U_i is the ultrasonic velocity

3.RESULTS AND DISCUSSIONS

Alcohols used for the present study 1-propanol, 1-butanol are highly polar aprotic. Alcohols usually exist in polymeric form. In the presence of polar molecules they dissociate into moments with the increase in order of alcohols, the tendency for intermolecular hydrogen bonding also increases. The association is stronger and we expect a larger variation in the parameters.

Table 1 Ultrasonic velocity of 1-propanol+methyl isobutyl ketone + benzene

Mole fraction		U_{EXP}	Theoretical Ultrasonic Velocity (m/s)				
x_1	x_3	(m/s)	U_{NR}	U_{IMR}	U_J	U_{IR}	U_R
0.0000	0.7001	1199.1	1197.1	1200.7	1323.1	1208.4	1204.6
0.1001	0.6005	1211.0	1199.8	1191.7	1326.7	1210.5	1206.6
0.2000	0.4997	1214.6	1202.6	1187.5	1329.0	1211.8	1207.5
0.2997	0.3984	1220.6	1205.9	1187.2	1332.6	1213.6	1203.9
0.3998	0.3001	1221.4	1209.3	1185.6	1335.3	1216.4	1212.5
0.4988	0.1999	1222.0	1213.2	1190.7	1339.4	1218.4	1216.2
0.6002	0.0998	1226.0	1217.8	1195.8	1343.1	1220.4	1217.1
0.6983	0.0000	1231.2	1222.7	1207.7	1349.9	1222.3	1214.1

Table 2 Ultrasonic velocity of 1-Butanol + methyl isobutyl ketone + benzene

Mole fraction		U_{EXP}	Theoretical Ultrasonic Velocity (m/s)				
x_1	x_3	(m/s)	U_{NR}	U_{IMR}	U_J	U_{IR}	U_R
0.0000	0.7001	1199.1	1197.1	1200.8	1332.1	1208.3	1204.6
0.1002	0.5999	1225.6	1202.6	1204.3	1329.3	1214.0	1212.2
0.2060	0.5000	1226.9	1208.5	1201.7	1335.4	1219.4	1214.6
0.3000	0.4000	1230.2	1214.6	1214.1	1341.6	1224.9	1214.6
0.3999	0.2999	1233.0	1221.3	1220.4	1348.5	1230.2	1226.8
0.4995	0.1972	1235.0	1228.7	1231.4	1356.1	1235.9	1228.1
0.5840	0.0863	1238.9	1237.6	1274.3	1366.4	1242.3	1238.7
0.7009	0.0000	1241.7	1244.5	1242.8	1373.0	1246.5	1239.6

The values of ultrasonic Velocities computed using Nomoto's(1958), U_{NR}, ideal mixing method (Van and Vangael,1955),U_{IMR}, Junjie (1984), U_J, Impedance relation method(Baluja and Parasania, 1995), U_{IR} and Rao's specific velocity method(Gokhale and Bhagavat, 1989), U_R together with experimental values for the systems 1-propanol, 1-butanol, mixed with methyl isobutyl ketone and benzene are presented in Table 1 and Table 2 and their corresponding variation with mole fraction are represented graphically in Figure 1 and Figure 2.

It can be seen from Tables 1 for the 1-propanol + methyl isobutyl ketone + benzene system; there is a less agreement between experimental and theoretical values calculated by Nomoto, ideal mixing method, impedance relation method and Roa's method but a good agreement among themselves. Higher variations are observed in Junjie's method.

Similarly for the 1-butanol + methyl isobutyl ketone + benzene system Table 2 there is less satisfactory agreement between the experimental and theoretical values computed by all the four methods but all the four computed methods agree with one another except Junjie method which shows large variations.

Table 3 and Table 4 gives the percentage of deviation for the different theoretically computed methods from experimental values and the molecular association parameter α for the system 1-propanol, 1-butanol, mixed with methyl isobutyl ketone in benzene and their corresponding variation with mole fraction are presented graphically in Figure 3 and Figure 4.

Table 3 Percentage of deviation of theoretical ultrasonic velocity with experimental value for the system: 1-Propanol + benzene+ Methyl isobutyl ketone

Mole fraction		U_{EXP}	Percentage Deviation(ΔU/U)					
x_1	x_3	(m/s)	U_{NR}	U_{IMR}	U_J	U_{IR}	U_R	α
0.0000	0.7001	1199.1	0.1667	0.1334	10.341	0.7755	0.4586	-0.0026
0.1001	0.6005	1211.0	0.9248	0.0159	9.5540	0.0412	0.3633	0.0326
0.2000	0.4997	1214.6	0.9879	2.1817	9.4187	0.2305	0.5845	0.0461
0.2997	0.3984	1220.6	1.2043	2.7363	9.1758	0.5734	1.3681	0.0570
0.3998	0.3001	1221.4	0.9906	2.9370	9.3253	0.4093	0.7286	0.0673
0.4988	0.1999	1222.0	0.7201	2.5613	9.6072	0.2945	0.4746	0.0542
0.6002	0.0998	1226.0	0.6688	2.4632	9.5513	0.4567	0.7259	0.1742
0.6983	0.0000	1231.2	0.6903	1.9087	9.6410	0.7228	1.3888	0.0392
			0.7941	1.8664	9.5767	0.4371	0.7615	

Table 4 Percentage of deviation of theoretical ultrasonic velocity with experimental value for the system: 1-Butanol + benzene+ Methyl isobutyl ketone

Mole fraction		U_{EXP}	PercentageDeviation(ΔU/U)					
x_1	x_3	(m/s)	U_{NR}	U_{IMR}	U_J	U_{IR}	U_R	α
0.0000	0.7001	1199.1	0.1667	0.1417	11.0916	0.7672	0.4586	-0.0028
0.1002	0.5999	1225.6	1.8766	1.7379	8.4611	0.9464	1.0933	0.0356
0.2060	0.5000	1226.9	1.4997	2.0539	8.8434	0.6112	1.0025	0.0423
0.3000	0.4000	1230.2	1.3166	1.3087	9.0554	0.4308	1.2680	0.0266
0.3999	0.2999	1233.0	0.9489	1.0218	8.5428	0.2270	0.5028	0.0207
0.4995	0.1972	1235.0	0.5101	0.2914	9.8056	0.0728	0.5587	0.0058
0.5840	0.0863	1238.9	0.1049	0.3712	10.2671	0.2744	0.0161	0.0074
0.7009	0.0000	1241.7	0.2254	0.0885	10.5742	0.3865	0.1932	-0.0076
			0.5930	0.5390	10.6085	0.4310	0.4460	

From these tables it is observed that Nomoto's relation shows a percentage deviation of (0.1 to 0.9) % in system [1-

propanol mixed with methyl isobutyl ketone in benzene] and (0.1 to 1.8) % in system [1-butanol, mixed with methyl isobutyl ketone in benzene]. Whereas the ideal mixing relation shows variation of (0.01 to 2.9) % for system [1-propanol, mixed with methyl isobutyl ketone in benzene] and (0.08 to 2.04) % for system [1-butanol, mixed with methyl isobutyl ketone in benzene]. For the Junjie's relation the corresponding percentage of deviation for system [1-propanol mixed with methyl isobutyl ketone in benzene] and system [1-butanol mixed with methyl isobutyl ketone in benzene] are as follows (9.1 to 10.3) % and (8.4 to 11.0) % respectively.

Figure 1 Variation of ultrasonic velocities with mole fraction for the system 1-propanol+methyl isobutyl ketone + benzene

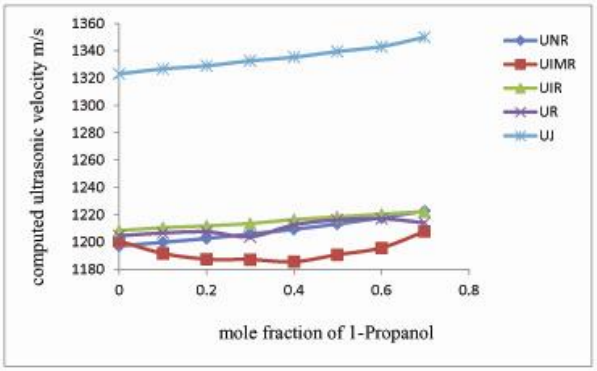
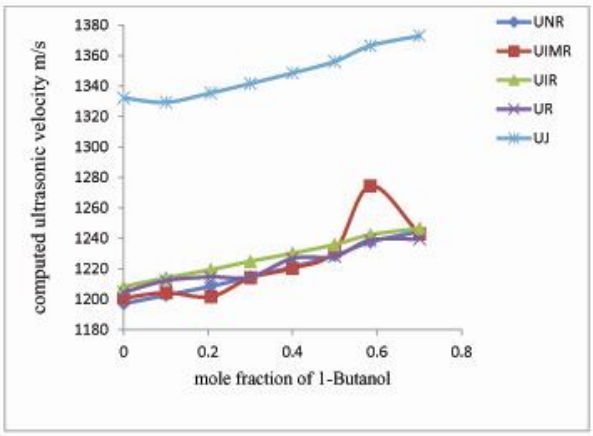


Figure 2 Variation of ultrasonic velocities with mole fraction for the system 1-Butanol+methyl isobutyl ketone + benzene



Similarly for impedance relation method, for system [1-propanol mixed with methyl isobutyl ketone in benzene] and for system [1-butanol mixed with methyl isobutyl ketone in benzene] the percentage of deviation are (0.04 to 0.77) % and (0.02 to 0.94) % respectively and that for Roa's relation method the percentage of deviation for the two systems are from (0.3 to 1.38) % and (0.01 to 1.2) %.

The limitations and approximation incorporated in these theories are responsible for the deviations of theoretical values for experimental values. In Nomoto's theory, it is supposed that the volume does not change on mixing. But on mixing two liquids, the interaction between the molecules of the two liquids takes place because of the presence of various types of forces such as dispersive forces, charge transfer, hydrogen bonding, dipole-induced dipole-dipole and dipole-induced dipole interaction. In Van Dael and Vangeel equation the deviation might be due to the compressibility of the components liquids in the present mixture.

The deviation in impedance and Rao's relation imply the non-additivity of acoustic impedance and Rao's velocity in liquid mixtures. Large deviation is observed in case of Junjie relation. Further this deviation is reported in the literature(Viswanatha Sharma *et al.*, 1999). Thus the observed deviation of both theoretical and experimental values show molecular interaction are taking place(Begum et al., 2012) between the unlike molecules and in liquid mixture.

Figure 3 Variation of Percentage of deviation of theoretical ultrasonic velocity with experimental value for different mole fraction for the system 1-propanol+methyl isobutyl ketone + benzene

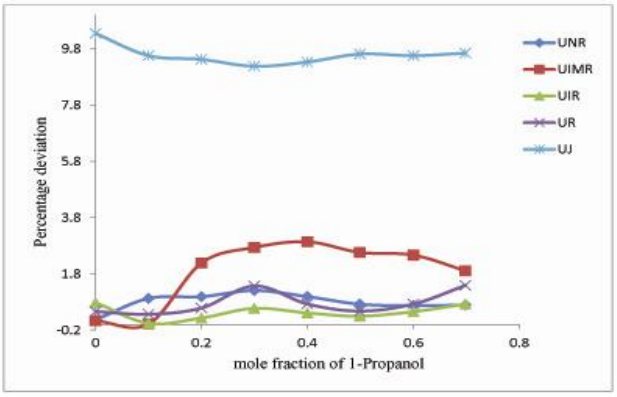
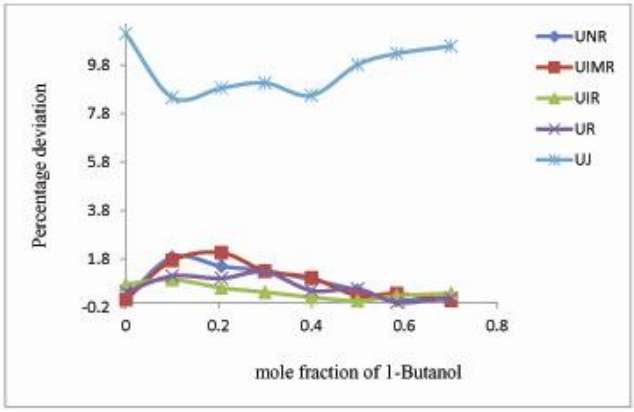


Figure 4 Variation of Percentage of deviation of theoretical ultrasonic velocity with experimental value for different mole fraction for the system **1-Butanol +methyl isobutyl ketone +**



There are high deviations in some intermediate concentration range suggesting the existence of strong tendency of association between components molecules as a result of hydrogen bond(Ramo Rao et al., 2005).Looking into the behavior of all two ternary mixtures, it can be understood that, positive percentage of deviation in velocity are attributed to the molecular associations.

The ratio U^2_{exp}/U^2_{imx} is an important tool to measure the non-ideality in the mixture especially in such cases where the properties other than ultrasonic velocity are known (Viswanatha Sharma *et al.*, 1999). The evaluated interaction parameters are positive for all systems, indicating stronger interaction between mixing molecules. Except for $X_1 = 0.0$ mole fraction which indicates the binary mixture of benzene and methyl isobutyl ketone) and for $X_2 = 0.7009$ (binary mixture of 1-butanol and benzene) indicating stronger interaction between mixing molecules. The negative value indicates the dominance of dispersion forces arising from the breakage of hydrogen bonds in the associates ie between

benzene and methyl isobutyl ketone and between benzene and 1-butanol. The specific percentage of deviation values are high in system 2 than that in system 1Table 3 and Table 4.

4.CONCLUSION

Data reveal that the ultrasonic study of the ternary mixture of the systems

1) 1-propanol + methyl isobutyl ketone + benzene
2) 1-butanol + methyl isobutyl ketone + benzene

Shows molecular association between the components are in the order 1-propanol < 1-butanol.

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