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Theoretical evaluation of sound velocity in Ternary liquid system

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ABSTRACT

Sound velocity values are evaluated from various theoretical models at 303K in the organic liquid systems and have been compared with the experimental values. The validity of Nomoto, Van Dael-vangeel Ideal mixture relation, Impedance dependence relation and collision factor theories have been checked and comparative study of the above models is made. The non-ideal behaviour of the system is explained on the basis of the molecular interactions of the constituents of the mixture.

Keywords: Ultrasonic velocity, ternary liquids, Nomoto's relation, molecular interactions.

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INTRODUCTION

Ultrasonic investigations provide extensive applications in characterizing thermodynamic and physico-chemical behaviour of liquid mixtures [1]. Theoretical estimation of ultrasonic velocity gives a better understanding of molecular arrangement in liquids [2]. Recently, thermodynamic and ultrasonic studies of molecular interactions have got considerable importance in developing theoretical models as well as its application in industry and engineering [3]. Several researchers carried out investigations on ultrasonic velocity with the theoretical relations of Nomoto's [4], Free length theory of Jacobson [5], Impedance dependence relation [6] and ideal mixing relation [7] in which, the results are interpreted in terms of molecular interactions. The theoretical values are compared with the experimental ultrasonic velocity values and the validity of this formulation for describing the ultrasonic response of these mixtures has been examined. The non-ideal behaviour of these systems has been explained in terms of interactions between their constituents.

EXPERIMENTAL

1-alkanols, benzene and anisole (Sd Fine chemicals, India) of AR grade of 99.5% purity were used as such without further purification. The mixtures were prepared by weight and were kept in special airtight bottles. The weighing was done on an electronic digital balance with a precision of ± 0.1 mg. The densities of pure liquids were measured using a single capillary pycnometer (made of borosil glass). The marks on the stem were calibrated with triple distilled water. The ultrasonic speeds in pure liquids were measured using single crystal, variable path ultrasonic interferometer (Mittal Enterprises, New Delhi Model M-82) operating at 3 MHz. The temperature of the solution was maintained constant within $\pm 0.01^\circ\text{C}$ by circulation of water from thermostatically regulated water bath through the water jacketed cell. The velocity measurements were precise to 0.5 ms^{-1} . The viscosity is determined using Ostwald viscometer which is calibrated at all the temperatures investigated using triply distilled water. In this method, the time of flow of a given volume of sample liquid, through a capillary is compared with that of a reference liquid of known density and viscosity. The viscosity of the sample liquid can be determined if the density of the same is known. The estimated accuracy in the measurement of viscosity is $\pm 0.1\%$.

Theory:

The experimental values U_{exp} of ultrasound velocity was compared with those obtained from the following relation [8].

Nomoto's relation:

Nomoto established an empirical formula for ultrasonic velocity in binary liquid mixtures on the assumption of linear dependence of the molar sound velocity on concentration in mole fractions and the additivity of molar volume as

$$U_{NR} = \left(\frac{X_1 R_1 + X_2 R_2 + X_3 R_3}{X_1 V_1 + X_2 V_2 + X_3 V_3} \right)^3 \quad (1)$$

Where X_1 , X_2 and X_3 are the mole fractions of the components, R_1 , R_2 and R_3 respective molar sound velocities and V_1 , V_2 and V_3 are the molar volumes respectively.

Where molar sound velocity

$$R = \frac{M}{\rho} U^{\frac{1}{3}} = V U^{\frac{1}{3}}$$

The molar volume

$$V = \frac{M}{\rho}$$

Impedance Dependence Relation (IDR)

The sound speed in the mixture is given by Impedance dependence relation (IDR) as

$$U_{IDR} = \frac{\sum_{i=1}^3 X_i Z_i}{\sum_{i=1}^3 X_i \rho_i} \quad (2)$$

Where z is the acoustic impedance and ρ is the density of the components in the mixture.

Ideal mixture relation (IMR)

$$U_{IMR} = \left(\frac{1}{X_1 m_1 + X_2 m_2 + X_3 m_3} \right)^{1/2} \left(\frac{X_1}{m_1 U_1^2} + \frac{X_2}{m_2 U_2^2} + \frac{X_3}{m_3 U_3^2} \right)^{-1/2} \quad (3)$$

The degree of molecular interaction α can be computed from the equation given under,

$$\alpha = \left(\frac{U_{exp}^2}{U_{IMR}^2} \right) - 1 \quad (4)$$

Collision Factor Theory (CFT)

$$U_{CFT} = U_{\infty} \left[\frac{(X_1 S_1 + X_2 S_2 + X_3 S_3) (X_1 B_1 + X_2 B_2 + X_3 B_3)}{V_m} \right] \quad (5)$$

Where,

Molar volume of mixture $V_m = \left[\frac{(X_1 m_1 + X_2 m_2 + X_3 m_3)}{\rho} \right]$

Actual Volume $B = 4/3 \pi r^3 N$

Molecular radius $r = \left(\frac{3b}{16\pi N} \right)^{1/3}$

Where,

U_∞ is the temperature dependent constant ($U_\infty = 1600 \text{ m s}^{-1}$),
 b is the Vander Waal's constant and N is the Avogadro Number.

Percentage Deviation

The modulus of percentage deviation [9] in sound velocity between the experimental and computed values are calculated as

$$\left(\frac{\Delta U}{U} \right) \% = \left(\frac{U_{\text{exp}} - U_{\text{theo}}}{U_{\text{exp}}} \right) 100 \quad (6)$$

Standard Percentage Error

The standard percentage error (e) is calculated using the relation

$$e = \left(\frac{\left(\sum \frac{\Delta U}{U} \right)^2 \%}{n} \right)^{1/2} \quad (7)$$

RESULTS AND DISCUSSION

The experimentally measured ultrasonic velocity values and the estimated ultrasonic velocity obtained from the various theoretical systems 1-propanol+benzene+anisole, 1-butanol+benzene+anisole, 1-pentanol+ benzene+ anisole taken up for this study are given in Table 1. The modulus of percentage deviation of ultrasonic velocity for Nomoto's relation (NR), Ideal Mixture Relation (IMR), Ideal Dependence Relation (IDR) , Collision Factor Theory(CFT), molecular interaction parameters(α) , the average percentage deviation and standard percentage error values are given in Table 2 for all the three systems.

Table 1: Values of experimental and theoretical ultrasonic velocity (U) at 303K

Mole fraction		Ultrasonic velocity (ms^{-1})				
x_1	x_3	U_{exp}	U_{NR}	U_{IMR}	U_{IDR}	U_{CFT}
System: 1-propanol (x_1) + Benzene (x_2) + Anisole (x_3)						
0.0000	0.6000	1340.0	1349.6	1317.2	1349.4	1342.0
0.1000	0.5000	1332.1	1322.8	1280.0	1331.7	1342.8
0.2000	0.4000	1325.7	1315.0	1252.2	1313.2	1326.0
0.3000	0.3000	1318.5	1296.0	1232.3	1293.9	1322.0
0.4000	0.2000	1300.4	1275.8	1219.3	1373.8	1308.4
0.5000	0.1000	1218.0	1254.2	1212.5	1252.7	1246.2
0.6000	0.0000	1215.1	1231.0	1211.6	1230.7	1227.5
System: 1-butanol (x_1) + Benzene (x_2) + Anisole (x_3)						
0.0999	0.5000	1336.8	1333.5	1296.5	1334.2	1349.5
0.1999	0.4000	1330.6	1316.9	1279.8	1318.5	1339.3
0.2999	0.2999	1323.4	1299.9	1266.6	1302.1	1340.5
0.4000	0.2000	1315.1	1282.4	1256.6	1285.0	1331.7
0.5001	0.0999	1240.3	1267.4	1249.6	1267.1	1276.3
0.5999	0.0000	1225.2	1246.0	1245.5	1248.5	1246.7
System: 1-pentanol (x_1) + Benzene (x_2) + Anisole (x_3)						
0.0999	0.5000	1314.3	1334.8	1305.0	1336.7	1357.3
0.2000	0.3999	1332.6	1320.1	1294.2	1323.5	1352.9
0.3000	0.3000	1324.8	1305.6	1284.6	1309.9	1359.2
0.4000	0.2001	1317.7	1291.2	1276.3	1295.6	1351.2
0.4999	0.0999	1289.5	1276.8	1269.2	1280.7	1314.7
0.6000	0.0000	1279.2	1262.6	1263.1	1265.2	1307.5

Table 2: Values of the Modulus of percentage deviation, Average percentage error and standard percentage error at 303K

	U_{NR}	U_{IMR}	U_{IDR}	U_{CFT}	α
System: 1-propanol (x_1) + Benzene (x_2) + Anisole (x_3)					
	0.72	1.70	0.70	0.15	0.03
	0.05	3.91	0.03	0.80	0.08
	0.81	5.54	0.94	0.02	0.12
	1.70	6.54	1.86	0.27	0.14
	1.89	6.24	2.05	0.61	0.14
	2.97	0.45	2.85	2.31	0.01
	1.31	0.29	1.28	1.02	0.01
APE	1.35	3.52	1.39	0.74	-
SPE	1.61	4.32	1.64	1.03	-
System: 1-butanol (x_1) + Benzene (x_2) + Anisole (x_3)					
	0.72	1.70	0.70	0.15	0.03
	0.25	3.01	0.19	0.95	0.06
	1.03	3.82	0.91	0.65	0.08
	1.78	4.29	1.61	1.29	0.09
	2.49	4.45	2.29	1.26	0.10
	1.70	1.66	1.90	1.75	0.03
APE	1.41	2.81	1.39	1.28	-

SPE	1.59	3.12	1.58	1.51	-
System: 1-pentanol (x_1) + Benzene (x_2) + Anisole (x_3)					
	0.71	1.71	0.70	0.14	0.04
	1.56	0.71	1.70	3.27	0.01
	0.94	2.89	0.68	1.53	0.06
	1.45	3.03	1.13	2.60	0.06
	2.01	3.14	1.68	2.54	0.07
	0.98	1.58	0.68	1.96	0.03
	1.30	1.26	1.09	2.21	0.03
APE	1.28	2.05	1.09	2.03	-
SPE	1.34	2.23	1.17	2.24	-

The variation of experimental and theoretical sound velocities with the concentration of alcohol in the mixtures under study for the three systems are represented in Figs.1 to 3. The perusal of the figures reveal good agreement between the experimental and calculated sound velocities, owing to the several assumptions and approximations made in the respective theories.

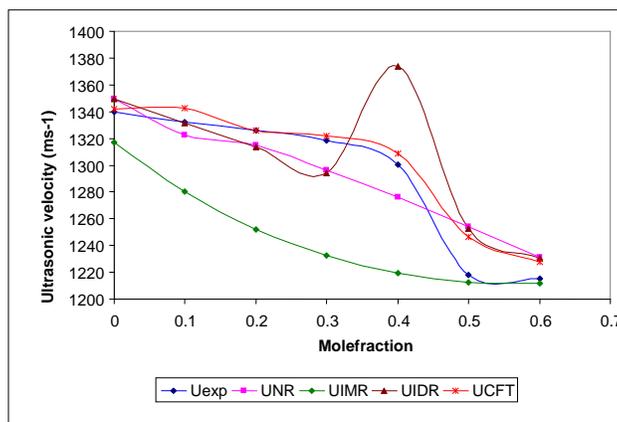


Fig. 1 Variation of experimental and theoretical ultrasonic velocity Vs mole fraction of 1-Propanol at 303K

The limitation and approximation incorporated in these theories are responsible for the deviation of theoretical from experimental values. In Nomoto’s theory, no interaction between the components of liquid mixtures has been taken into account as it is supposed that the volume doesn’t change on mixing. Similarly, the assumption for the formation of ideal mixing relation is that the ratios of specific heats of ideal mixtures and the volumes are equal by not taking molecular interactions into consideration. Various types of forces such as dispersion forces, charge transfer, hydrogen bonding, dipole-dipole and dipole- induce dipole interactions are operative due to interactions when liquids are mixed. Thus, the observed deviation of theoretical values of velocity from the experimental values shows that the molecular interactions taking place between the unlike molecules in the liquid mixture [10].

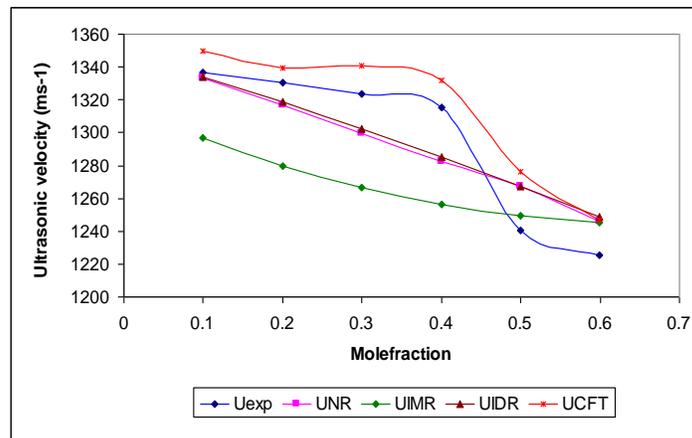


Fig. 2 Variation of experimental and theoretical ultrasonic velocity Vs mole fraction of 1-Butanol at 303K

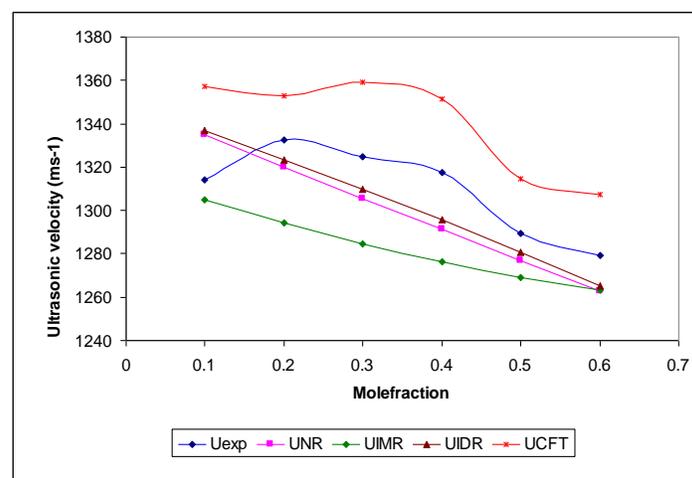


Fig. 3 Variation of experimental and theoretical ultrasonic velocity Vs mole fraction of 1-Pentanol at 303K

It is observed from the Table 1 that Nomoto's relation predicts a good agreement of sound velocity with the experimental values in ternary mixtures of 1- propanol and 1- pentanol with benzene and anisole but fails to do so in the 1-butanol+benzene+anisole system. The Ideal Mixture Relation (IMR) yields a fair estimation of sound velocity for 1-butanol and 1-pentanol with benzene and anisole whereas a poor agreement for the other system. Impedance dependence value closely follows the experimental value in 1-pentanol+benzene+anisole mixture. It also estimates the sound velocity values of the other two systems to a certain degree of accuracy. The collision factor model of sound velocity confirms well with the experiment in ternary system of 1-propanol system. It fails to confirm with the values of 1-pentanol system whereas the other system is better compared to the above said systems.

Thus from the comparison of experimental velocity values with theoretical models, it is clear that the collision factor theory is best suited for system I and II and impedance dependence relation for system III. Ideal mixing relation is not satisfactory [11].The percentage

of deviation of the theoretical ultrasonic velocity values from the experimental values are shown in Table 2. We infer from the Table 2 that for 1-propanol and 1-butanol systems, the theoretical ultrasonic velocity values based on collision factor theory gives less percentage of deviation than that of other theories. For 1-pentanol system, the theoretical velocity values based on impedance dependence relation gives less percentage of deviation than the other theoretical models [12]. On the whole, all the theoretical models fairly predict that the ultrasonic velocities are reasonably close to the experimental values for the three ternary mixtures reported in this work, thus showing the validity of these theoretical models.

CONCLUSION

The above discussions lead to the following conclusions:

1. Among the four theories studied, CFT is found to be best suited for the system I and II and IDR is best suited for the system III.
2. The positive α values present in all the three systems confirm the presence of strong interaction between the components of the mixtures.

REFERENCES

- [1] Anwar Ali, Anil kumar Nain, Narender kumar and Mohammed Ibrahim. J Pure Appl Ultrason 2002; 24:27-35.
- [2] Agnishotri PK and CS. Adgaonhar Ultrasonics 1989; 27: 248-251.
- [3] AK Gupta, Krishna Kumar and Birendra Kumar Karn. J Ind Council Chem 2009; 26(1):77-81.
- [4] Nomoto O. J Phys Soc Japan 1958; 13:1528.
- [5] Jacobson. J Chem Phys 1952; 20:927.
- [6] Arul G and Palaniappan L. J Acoust Soc Ind 2000; 28:393-395.
- [7] Van Dael and Vangeel E. Proceedings of the first and international conference on Calorimetry thermodynamics. Warsaw 1969; 555.
- [8] Sumathi T, Abeetha K. E J Chem 2011; 8(1):252-256.
- [9] Palani R and Meenakshi K. I J Chem 2007; 46A: 252.
- [10] Raju K, Karpagavalli K. J convergence in Eng Tech and Sci 2005; 1:32-35.
- [11] Jajoo SN, Adgaonkar CS and Deogaonkar VS. I J Pure Appl Phys 1983; 21:65.
- [12] Prabakar S and Rajagopal K. J Pure Appl Ultrason 2005; 27:41-48.