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Computation of Ultrasonic Speed in Binary Liquid Mixture of Acetone and Carbon tetrachloride using Empirical Theories at Different Temperatures

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Abstract

Experimental ultrasonic velocities of binary liquid mixture of acetone and carbon tetra chloride at temperatures 286.15 K, 289.15 K and 293.15 have been evaluatedat 2 MHz as a function of molar concentrations. The experimental values were compared with various theories for analysis of ultrasonic velocity in binary liquid mixtures such as Nomoto theory (NOM), ideal mixing relation (IMR) of Van Dael andVangeel, Impedance Relation (IDR), Rao's Specific Velocity Method (Rao) and Junjie's relations (JR). Chi-square test and average percentage error were applied to investigate the relative applicability of these theories to the present systems. The variation of thermo acoustical parameters of the systems with the mole fraction has been discussed in term of molecular interactions.

Key words : Ultrasonic velocity, Chi-square test, Average percentage error, Molecular interaction and thermo-acoustical parameters.

Introduction

Ultrasonic velocityplays a very import role in determining the physico-chemical behaviour of liquid mixtures and it has vast applications in the industry. Investigation of sound in liquids has been

carried by many researchers[1-4] from several years. Ultrasonic velocities in liquid mixtures have been calculated and compared with experimental values using various theories[5,6]. Measurement of ultrasonic velocities gives valuable information about the Physio-chemical behaviours of liquids and their mixtures[7-8]. Comparison of evaluated theoretical velocities with those obtained experimentally is expected to reveal the nature of interaction between component molecules in the mixtures of different molar concentration. Such theoretical study is useful in determining a comprehensive theoretical model for a specific liquid mixture. They are also valuable in testing various theories of liquid state. Many researchers compared the experimental values of ultrasonic velocities with theoretically evaluated values for organic liquid mixtures using different theoretical models like Nomoto theory[9], Ideal mixing relation[10], Impedance relation[11], Rao's specific velocity theory[12] and Junjie's relation[13]. The goal of the present investigation is to compare the experimentally determined ultrasonic velocity in binary liquid mixtures with the values observed using different theoretical models like Nomoto, Ideal mixing relation Impedance relation of Van Dael andVangeel, Rao's specific velocity and Junjie's relations. In the present investigation binary liquid mixtures made from Acetone and Carbon Tetrachloride are used to study the extent of interactions between the dissimilar molecules. The results are explained and discussed in terms of intermolecular interactions occurring in these binary systems. The deviation in the variation of average percentage error (APE) and Chi-square test for goodness of fit, from unity have also been evaluated to further explain the non-idealistic behaviour of the systems.

Materials and Methods :

The liquid mixtures of Acetone in Carbon Tetrachloride of various mole concentrations in terms of mole fractions were prepared by taking AR grade chemicals. All the liquids used were purified by the standard methods. The mixtures were preserved in well-stopper conical flasks. After the thorough mixing of the liquids, the flasks were left undisturbed to allow them to attain thermal equilibrium. In all the mixtures the mole fractions in of Acetone has been increased from 0.0 to 1.0 in Carbon Tetrachloride. The ultrasonic velocities were measured by using a frequency ultrasonic pulse interferometer (Model No. F-83, Mittal Enterprises. New Delhi). It consists of a high range frequency generator (2MHz) and a measuring cell. The measurements of ultrasonic velocities were made at a fixed frequency of 2MHz. Temperature was controlled by circulating water around the liquid cell from thermostatically digital controlled constant temperature water bath and the temperature was fixed constant. The densities of pure liquids and liquid mixtures were measured by using a specific gravity bottle with an accuracy of ±0.5%.

Various theories used for analysis of ultrasonic velocities in binary liquid mixtures.

1. Nometo established an empirical relation for ultrasonic velocity is binary liquid mixture as:

$$U_{Nom} = \left(\frac{x_1 R_1 + x_2 R_2}{x_1 V_1 + x_2 V_2}\right)^3 \quad (1)$$

where $R = \frac{Mu^{\frac{1}{3}}}{\rho_1}$ is molecular sound velocities, x_1 and x_2 are the mole fraction of first and second

compound of the liquid mixture and V is molar volume

2. Impedance dependent relation :

$$U_{IDR} = \sum xiZi \Big/ \sum xi\rho i \tag{2}$$

Where x_i is the mole fraction, ρ_i is the density of the mixture and Z_i is the acoustic impedance.

3. Rao's specific velocity :

$$U_{Rao} = \sum (x_i\, r_i \rho_i)^3 \tag{3}$$

x_i is the mole fraction, ρ_i is the density of the mixture.

4. Zhang-Junjie relation:

$$U_{JR} = \frac{x_1 v_1 + x_2 v_2}{(x_1 M_1 + x_2 M_2)^{\frac{1}{2}}} \left[\frac{x_1 v_1}{\rho_1 v_1^2} + \frac{x_2 v_2}{\rho_2 v_2^2}\right]^{-1/2} \tag{4}$$

Where x_1 and x_2 is the mole fractions first and second comports of mixture, ρ_1 and ρ_2 is the densities of the constituents' components.

5. Van Dael andVangeel ideal mixing relations :

$$U_{IMR} = \left(\frac{x_1}{M_1 V_1^2} + \frac{x_2}{M_2 V_2^2}\right)^{-\frac{1}{2}} (x_1 M_1 + x_2 M_2)^{-\frac{1}{2}} \tag{5}$$

Where M_1 and M_2 are molecular weights of constituent components, v_1 and v_2 are the ultrasonic velocities of individual components. The ultrasonic velocities on the basis of above theories are evaluated and is verified by experimental determination, which would help us in finding the appropriate theory applicable to the mixture under study. The following tests are the adopted for examining the accuracy of the results.

6. Chi-square test for goodness of fit :
According to Karl Pearson chi-square value is evaluated for binary liquid mixture under study using the formula as

$$\chi^2 = \sum_{i=1}^{n} \frac{(U_{mix\,(Obs)} - U_{mix\,(cal)})^2}{(U_{mix\,(cal)})} \tag{6}$$

Where n is the number of data used.

7. Average percentage error :

$$APE = \frac{1}{n} \sum \frac{[U_{mix\,(Obs)} - U_{mix\,(cal)}]}{(U_{mix\,(Obs)})} * 100 \tag{7}$$

Results & discussion

The values of ultrasonic speed obtained fromvarious theories for binary liquid mixtures of

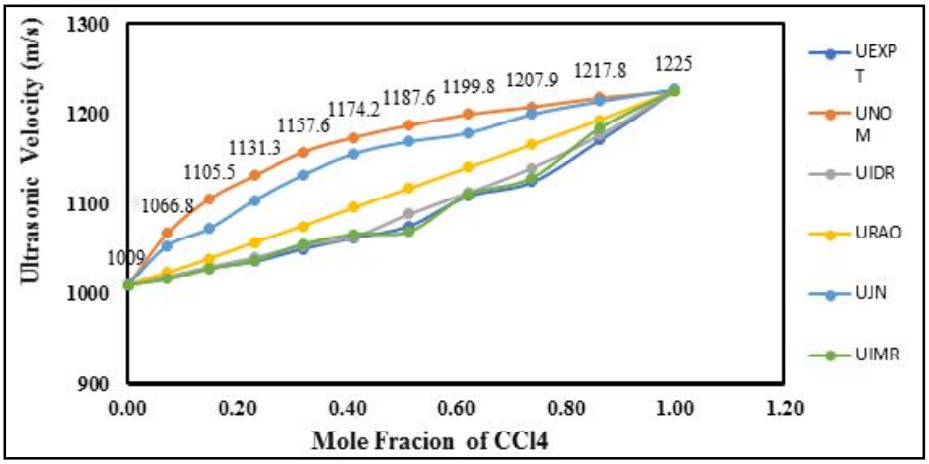

Fig. 1: Variation of Experimental and Theoretical velocity with respect to mole fraction at 286.15K

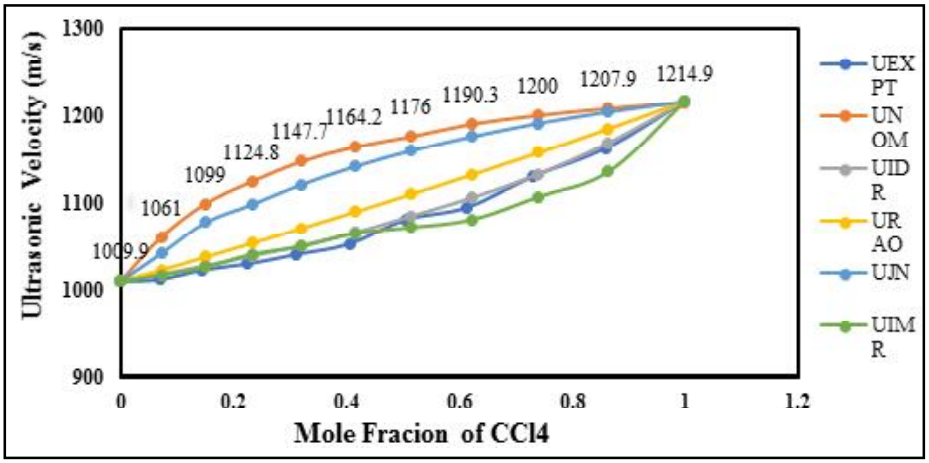

Fig. 2: Variation of Experimental and Theoretical velocity with respect to mole fraction at 289.15K

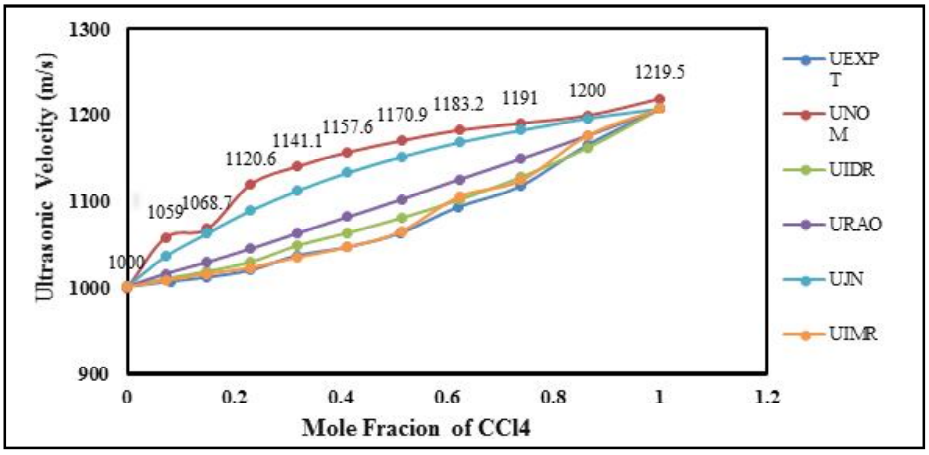

Fig. 3: Variation of Experimental and Theoretical velocity with respect to mole fraction at 293.15K

Table 1: Experimental and theoretical values of speed of sound for Acetone and Carbon tetrachloride at temperature 286.15K

Mole Fraction	U_{EXP}	U_{NOM}	U_{IDR}	U_{RAO}	U_{JR}	U_{IMR}
0.0000	1010	1010.0	1010.0	1010.0	1010.0	1010
0.0725	1018	1006.8	1018.9	1023.8	1053.2	1016
0.1502	1029	1105.5	1030.0	1039.2	1072.4	1028
0.2326	1036	1131.3	1040.0	1057.1	1103.8	1037
0.3204	1050	1157.6	1053.6	1075.3	1132.0	1055
0.4143	1062	1174.2	1063.2	1095.5	1156.0	1066
0.5148	1075	1187.6	1088.1	1117.0	1169.5	1069
0.6227	1108	1199.8	1112.0	1140.5	1178.9	1110
0.7395	1124	1207.9	1140.0	1166.2	1200.0	1129
0.8642	1171	1217.8	1176.9	1194.0	1214.0	1185
1	1226	1226.0	1226.0	1226.0	1227.0	1226
APE		-6.49	-0.41	- 1.97	-5.10	0.184
χ^2		62.76	0.31	6.62	41.52	0.26

Table 2: Experimental and theoretical values of speed of sound for Acetone and Carbon tetrachloride at temperature 289.15K

Mole Fraction	U_{EXP}	U_{NOM}	U_{IDR}	U_{RAO}	U_{JR}	U_{IMR}
0.00	1010	1009.9	1010.0	1010.0	1010.0	1010
0.0703	1012	1061.0	1018.3	1022.9	1042.0	1017
0.1455	1023	1099.0	1027.9	1037.9	1077.5	1026
0.226	1030	1124.8	1039.0	1053.7	1098.0	1041
0.3124	1041	1147.7	1051.0	1070.9	1121.3	1050
0.4053	1053	1164.2	1066.0	1089.5	1141.8	1065
0.5054	1081	1176.0	1085.0	1110.0	1160.0	1072
0.6139	1095	1190.3	1106.0	1132.6	1176.0	1081
0.7317	1131	1200.0	1133.0	1157.6	1191.0	1107
0.8599	1163	1207.9	1169.0	1184.9	1204.0	1136
1	1216	1216.0	1216.0	1216.0	1216.0	1216
APE		-6.25	-0.55	-1.95	-4.91	0.29
χ^2		56.98	0.55	5.95	46.08	1.77

Table 3: Experimental and theoretical values of speed of sound for Acetone and Carbon tetrachloride at temperature 293.15K

Mole Fraction	U_{EXP}	U_{NOM}	U_{IDR}	U_{RAO}	U_{JR}	U_{IMR}
0.0000	1002.0	1002.0	1002.0	1002.0	1002.0	1002
0.0805	1008.0	1059.0	1011.3	1017.1	1037.0	1009
0.1489	1012.8	1068.0	1019.7	1030.3	1063.3	1017
0.2308	1021.0	1120.6	1030.6	1045.9	1090.0	1024
0.3183	1038.0	1141.1	1049.7	1064.0	1113.0	1036
0.4119	1047.6	1157.6	1064.3	1082.6	1133.8	1048
0.5123	1064.0	1170.9	1081.3	1102.9	1152.0	1066
0.6204	1094.0	1183.2	1102.5	1125.8	1168.8	1106
0.7369	1118.0	1191.0	1128.8	1150.0	1182.9	1125
0.8631	1166.0	1200.0	1162.8	1176.9	1196.5	1177
1	1207.6	1207.6	1207.6	1207.6	1207.6	1207.6
APE		-6.2	-0.69	-1.92	-4.82	-0.32
χ^2		56.03	0.98	6	34.92	0.31

acetone and carbon tetrachloride havebeen recorded in the Tables to 1 to 3 at 286.15 K, 289.15K and 293.15K respectively. The variation of Experimental and Theoretical ultrasonic velocity with respect to mole fraction of CCl4 in acetone at 286.15K, 289.15K and 293.15k are shown in Fig. 1, 2 and 3 respectively.

We have used the experimental data for the comparison of theoretical ultrasonic velocities obtained from various theories asreported earlier. A close perusal of Tables 1 to 3 reveals that the computed ultrasonic speed using impedance relation (IDR) and theory of ideal mixingrelation (IMR) compares well with our own experimental data. The percentage deviations between experimental values and theoretical predictions have also been reported in Tables 1 to 3.

The data reveals that the velocities computed from Ideal mixing relation (IMR) and Impedance relation (IDR) exhibitmore satisfactory agreement with the experimental values in the temperature range 286.15K to 293.15K than otherapproaches in the binary systems. It is observed that the experimental values show deviation with the theoreticalvalues of ultrasonic velocities which confirms the existence of molecular interactions[14-15]. This may be due tointeractions occurring between the hetero molecules of the binary systems. Higher deviations are observed in Nomoto and Junjie's theoriesand slight variations in Rao's relation. There are higher variations in some intermediate concentration rangesuggesting the existence of strong tendency of association between component molecules as a result of dipole-dipoleinteractions. However, there is reasonably a good agreement between the experimental and theoretical velocities of Van Dael and Vangeel's ideal mixing relation

and Impedance relation. 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. Similarassumptions have been made for the formation of ideal mixing relation according to which the ratios of specific heats of ideal mixtures and thevolumes are also equal. Again no molecular interactions are taken into account. But upon mixing, interactionsbetween the molecules occur because of the presence of various types of forces such as dispersion forces, chargetransfer, hydrogen bonding, dipole-dipole and dipole-induced dipole interactions. Thus, the observed deviation oftheoretical values of velocity from the experimental values shows that the molecular interactions are taking place between the unlike molecules in the liquid mixtures. Similar predictions have been made by Parmar *et al*.,[16-17] in context of the strength of molecular interactions and prediction of the probable associative molecular species in the liquid mixtures. Similar study has been made by Padmanaban *et al*.,[18] to predict the specific choice of theoretical model that could give the closest thermoacoustic property values for ethanol-based binary mixtures.

Conclusions

Ultrasonic velocities predicted using NOM, IMR, IDR, RAO and JR were compared withexperimentally measured velocity values at different temperatures from 286.15 K- 293.15K for the binary mixture of acetone and carbon tetrachloride. It may be concluded that ideal mixing relation of Van Dael and Vangeel is best suited for the binary mixtures of acetone and carbon tetrachloride at allthetemperatures. The observed deviation of theoretical values of velocity from the experimentalvalues is attributed to the presence of intermolecular interactions in the system studied.

The results of this study are expected to be useful in predicting the suitable molecular proportions that can be suited for industrial application. The results of the present study will provide insights and inference on knowing the best or most suited theoretical model that could predict the closest values of thermo-acoustic parameters for binary liquid mixtures.

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