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Research paper

A Comparative Study of Experimental and Theoretical Ultrasonic Velocity of Binary Liquid Mixtures Using Mathematical Methods

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Abstract

A comparative study of ultrasonic velocities of binary liquid mixtures such as O-cresol+carbon tetrachloride, anisicaldehyde+methylacetate, anisicaldehyde+ethylacetate, having industrial applications are analysed at temperature 303K for different concentrations [0 to 1%]. In the present study experimental values are taken from literature and there values are compared with theoretical values obtained by various mathematical equations such as Nomoto's relation, VandealVangeal formula, Impedance relation, Rao's specific relation. Thus, the present study reveals the nature of interaction between component molecules in the mixtures and enables us to identify a suitable mathematical model for predicting the ultrasonic velocity various binary liquid mixtures.

Keywords: *Binary liquids; Impedance relation; Nomoto's relation; Rao Specific relation; Ultrasonic velocity; Vand-deal and Van-Geal.*

1. Introduction

In recent years, there has been a continuous improvement in the experimental investigation of excess thermodynamic properties of liquid mixtures. Particularly, ultrasonic study of liquid mixtures has gained much importance in assessing the nature of molecular interactions present in the mixtures. Experimental and theoretical ultrasonic velocity studies in liquids and polymer solutions have been the subject of research in recent years. The experimental ultrasonic velocity values of O-Cresol with carbon tetrachloride, anisicaldehyde + methylacetate, anisicaldehyde + ethylacetate are compared with their theoretical values obtained by using various mathematical methods like Nomotto's Relation, Vandeal and Vangeal Relation, Impedance Relation and Rao's specific sound velocity. The most accurate mathematical method is identified using Average Percentage Error (APE).

2. Methods and Materials

The binary mixtures are prepared by dissolving O-Cresol with Carbon tetrachloride, anisicaldehyde with methylacetate and anisicaldehyde with ethylacetate to get desired concentrations. Magnetic stirrer [REMI make] was used for this purpose at a rate of 1000 rpm. Density values are measured using specific gravity method. The mass of the liquid was measured using a K-ROY make Electronic balance, with an accuracy of ±0.001gm. The ultrasonic velocity measurements are performed using Mittal make single frequency ultrasonic interferometer at 2 MHz (F-81 model) (uncertainty ± 0.01m/s).

3. Results and Discussion

3.1. Evaluation of Ultrasonic velocity

In recent years, measurement of ultrasonic velocity found extensive application in determining the physicochemical behavior of liquid mixtures. Theoretical evaluation of ultrasound velocity gives a better understanding of molecular arrangement in liquids [1-3]. In the present study, the experimental ultrasonic velocity values of O-Cresol with carbon tetrachloride, anisicaldehyde + methylacetate, anisicaldehyde + ethylacetateare compared with their theoretical ultrasonic velocities by Nomotto's relation (U_{Nom}), Vandeal Vangeal (U_{IMR}) relation, Impedance relation (U_{IR}) and Rao's specific sound velocity relation (U_R) as given below.

Nomotto's relation

On assuming the additivity of molar sound velocity (R) and no volume change on mixing, Nomotto established the following relation for a liquid mixture.

$$U_{NOM} = \left[\frac{X_1 R_1 + X_2 R_2}{X_1 V_1 + X_2 V_2} \right]^3 \quad (1)$$

Where, R is molar sound velocity, X_1 and X_2 are the mole fractions of 1st and 2nd components of the liquid mixture and V is molar volume. The molar sound velocity can be determined using the formula

$$R_1 = (M_1/d_1)U_1^{1/3} \quad (2)$$

$$R_2 = (M_2/d_2)U_2^{1/3} \quad (3)$$

where, M_1 and M_2 are the effective molecular weight of the 1st and 2nd components, d_1 and d_2 are the densities of the 1st and 2nd components and U_1 and U_2 are the ultrasonic velocities of the 1st and 2nd components.

Van Deal and Van Geal ideal mixing relation

Van Deal and Van Geal proposed the following expression for the estimation of sound velocity U_{IMR} in an ideal mixture using the sound velocities in the pure components.

$$U_{IMR} = \left[\frac{1}{\left(X_1M_1 + X_2M_{21}\right)^{1/2}}\right]\left(\frac{1}{\left(\frac{X_1}{M_1U_1^{\,2}} + \frac{X_2}{M_2U_2^{\,2}}\right)^{1/2}}\right) \quad (4)$$

where, X_1 and X_2 are the mole fractions of 1st and 2nd components of the liquid mixture, M_1 and M_2 are the effective molecular weight of the 1st and 2nd components, d_1 and d_2 are the densities of the 1st and 2nd components and U_1 and U_2 are the ultrasonic velocities of the 1st and 2nd components.

Impedance relation

Impedance relation is given by

$$U = \frac{\sum X_iZ_i}{\sum X_id_i} \quad (5)$$

Where, X_i, Z_i and d_i and $Z_i = U_i\ d_i$ are the mole fractions of the liquid mixture, specific acoustical impedance of the liquid mixture and density of liquid mixture.

Rao's specific relation

The Rao's Specific Sound velocity relation for determination of ultrasonic velocity in binary liquid mixture can be given as

$$U = \left(\sum X_ir_id_i\right)^3 \quad (6)$$

Where, r_i is the Rao's specific sound velocity and Z_i is the acoustical impedance. Rao's specific sound velocity can be calculated using the relation

$$r_i = U_i^{1/3} \,/\, d_i \quad (7)$$

3.2 Average Percentage Error

The average percentage error of deviation is calculated by the following formula

$$APE = \frac{1}{n}\sum\left[\left(\frac{U_{\exp} - U_{cal}}{U_{\exp}}\right)\right]*100 \quad (8)$$

The experimentally measured ultrasonic velocity and the estimated ultrasonic velocity from various mathematical models like Nomotto, Vandeal Vangeal, Impedance Relation and Rao's Specific Velocity Method for the binary liquid mixture O-Cresol with Carbon tetrachloride at five different concentrations at 303K are presented in the Table 1. From Table 1, it is observed that the experimental values of ultrasonic velocity increases with increase in concentration. The molecular association is responsible for this increasing trend. Similar trend is observed in Nomotto relation method, Impedance relation and Rao's specific velocity method. The ultrasound velocities obtained from Nomotto's relation method and Rao's specific sound velocity values are almost same [4-6]. The limitations and approximations incorporated in these theories are responsible for the deviations of theoretical values from experimental values. Table 2 shows the variation of percentage of deviation with respect to the composition of O-Cresol with Carbon tetrachloride at 303 K. In this system, it is understood that the percentage of deviation is more in Impedance relation (IMP) than Rao's specific relation (RAO) than Van-Deal and Vang-Geal (VV) than Nomotto's relation. i.e, IMP>RAO>VV>NOM. In Nomotto's relation only negligible deviation to experimental values is observed when compared to other methods. The experimentally measured ultrasonic velocity and the estimated ultrasonic velocity from various mathematical models for the binary liquid mixture anisic aldehyde (AA) +methyl acetate (MA) at five different concentrations at 303K are presented in the Table 2. From Table 3, it is observed that the experimental values of ultrasonic velocity increases with increase in concentration. The molecular association is responsible for this increasing trend. Similar trend is observed in Nomotto's relation method, Impedance relation and Rao's specific velocity method. The ultrasound velocities obtained from Nomotto's relation method and Rao's specific sound velocity values are almost same.

Table 1: Experimental and mathematical values of ultrasound velocity for O-cresol with Carbon tetrachloride

Conc (%)	EXP	NOM	VV	RAO	IMP
0.0154	971	1190	1150	1183	1151
0.0341	958	1289	1248	1282	1249
0.0571	996	1347	1312	1342	1312
0.1239	1116	1412	1390	1409	1390
0.175	1171	1432	1416	1430	1416
0.2482	1294	1447	1436	1446	1436
0.3614	1321	1460	1453	1459	1453
0.5601	1403	1470	1466	1469	1466

Table 2: Average percentage values of O-cresol with Carbon tetrachloride

Conc(%)	EXP	%NOM	%VV	%RAO	%IMP
0.0154	971	-22.55	-18.49	-21.80	-18.51
0.0341	958	-34.58	-30.3	-33.84	-30.33
0.0571	996	-35.22	-31.67	-34.63	-31.70
0.0861	1081	-28.13	-25.49	-27.71	-25.52
0.1239	1116	-26.49	-24.51	-26.18	-24.53
0.2482	1294	-11.8	-10.98	-11.72	-10.99
0.3614	1321	-10.48	-9.94	-10.40	-9.95
0.5601	1403	-4.77	-4.53	-4.73	-4.53
APE		-21.8	-19.7	-21.5	-19.6

Table 3: Experimental and mathematical values of ultrasound velocity for anisic aldehyde (AA) + methyl acetate (MA)

Conc(%)	EXP	NOM	VV	RAO	IMP
0.0685	1157	1145	1103	1171	1142
0.1420	1200	1186	1104	1230	1179
0.2210	1240	1227	1108	1285	1218
0.3062	1281	1269	1118	1338	1259
0.3984	1322	1312	1134	1387	1301
0.4983	1361	1357	1160	1432	1345
0.6071	1403	1402	1200	1471	1391
0.7259	1445	1448	1263	1502	1440

Table 4, illustrates the variation of percentage of deviation for binary mixture anisic aldehyde (AA) +methyl acetate (MA) at 303K. It is understood that percentage deviation is RAO>NOM>IMP>VV. In Van-Deal and Van Geal relation only negligible deviation to experimental values is observed when compared to other methods. The experimentally measured ultrasonic velocity and the estimated ultrasonic velocity from various mathematical models for the binary liquid mixture anisic aldehyde

(AA) + methyl acetate (MA) at five different concentrations at 303K are presented in the Table 5. Table 6, illustrates the variation of percentage of deviation for binary mixture anisic aldehyde (AA) + ethylacetate (EA) at 303K. It is clear that the variation of percentage of deviation which is RAO>IMP>NOM>VV. In Van-Deal and Van-Geal relation only negligible deviation to experimental values is observed when compared to other methods.

Table 4: Average percentage values of anisic aldehyde (AA) + methyl acetate (MA)

Conc(%)	EXP	%NOM	%VV	%RAO	%IMP
0.0685	1157	-0.95	-4.61	1.24	-1.26
0.1420	1200	-1.14	-7.99	2.54	-1.68
0.2210	1240	-1.04	-10.64	3.64	-1.76
0.3062	1281	-0.87	-12.71	4.46	-1.70
0.3984	1322	-0.74	-14.21	4.90	-1.60
0.4983	1361	-0.33	-14.74	5.20	-1.16
0.6071	1403	-0.10	-14.43	4.81	-0.84
0.7259	1445	-0.19	-12.60	3.97	-0.37
0.8563	1496	-0.04	-8.82	2.12	-0.37
AVG		-0.6	-11.2	3.65	-1.2

Table 5: Experimental and mathematical values of ultrasound velocity for anisaldehyde (AA) + ethyl acetate (EA)

Conc(%)	EXP	NOM	VV	RAO	IMP
0.0832	1170	1160	1128	1184	1165
0.1695	1215	1199	1138	1243	1208
0.2592	1259	1239	1153	1298	1251
0.3524	1303	1279	1172	1350	1293
0.4494	1342	1321	1198	1397	1335
0.5504	1381	1364	1232	1440	1377
0.6557	1421	1407	1277	1476	1419
0.7655	1462	1451	1337	1506	1461
0.8802	1503	1497	1421	1528	1502

Table 6: Average percentage values of anisic aldehyde (AA) + ethyl acetate (EA)

Conc(%)	EXP	%NOM	%VV	%RAO	%IMP
0.0832	1170	-0.85	-3.54	1.24	-0.422
0.1695	1215	-1.30	-6.27	2.31	-0.562
0.2592	1259	-1.63	-8.45	3.06	-0.688
0.3524	1303	-1.77	-10.01	3.60	-0.726
0.4494	1342	-1.55	-10.74	4.10	-0.498
0.5504	1381	-1.26	-10.81	4.22	-0.275
0.6557	1421	-0.99	-10.16	3.84	-0.147
0.7655	1462	-0.70	-8.50	2.99	-0.076
0.8802	1503	-0.41	-5.43	1.67	-0.072
AVG		-1.2	-8.2	3	-0.39

4. Conclusion

The experimental ultrasonic velocity values of binary liquid mixtures such as O-Cresol with carbon tetrachloride, anisicaldehyde+methylacetate, anisicaldehyde+ethylacetateare compared with their theoretical ultrasonic velocity values for different concentrations at a temperature 303K. From these it may be concluded that the binary mixtures anisicaldehyde + methylacetate, anisicaldehyde + ethylacetateshowed Vandeal & Vangeal relation as the best suitable method for calculating the speed of ultrasound waves in the liquid systems.

5. References

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