Theoretical Evaluation of Ultrasonic Velocities in Ternary Liquid Mixtures of Dibutylether + Toluene + 1-Alkanols at 303K

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Abstract: A comparison of ultrasonic velocity evaluated from Nomoto's relation, Van Deal- Vangeel ideal mixtures relation, impedance dependence relation and collision factor theories with experimental values have been made in three ternary systems of 1-alkanol with common binary mixture of toluene and dibutylether at 303 K. The relative applicability of these theories to the present systems has been checked and discussed.

Keywords: Ternary mixture, Ultrasonic velocity, Molecular interaction, Theoretical evaluation.

Introduction

The ultrasonic velocity measurement plays an important role in understanding the molecular interaction between the components of the mixture and provides an insight into the physico-chemical properties of liquid mixtures such as molecular association and dissociation as well as the strength of interaction between the components¹⁻². In order to get more information, an attempt has been made to correlate the experimental findings with those predicted theoretically on the basis of molecular models³⁻⁶. Further, the best suitable theory for the given molecular system understudy is also done by calculating the average percentage error. The present work includes

System I	1-Propanol + Toluene + Dibutylether (DBE)
System II	1-Butanol + Toluene + Dibutylether (DBE)
System III	1-Pentanol + Toluene + Dibutylether (DBE)

Experimental

The chemicals used in the present work were analytical reagent (AR) and spectroscopic reagent (SR) grades with minimum assay of 99.9%. In all systems, the various concentrations

of the ternary liquid mixtures were prepared in terms of mole fraction, out of which, the mole fraction of the second component toluene ($X_2=0.4$) was kept fixed while the mole fractions of the remaining two components 1-alkanols (X_1) and DBE(X_3) were varied from 0.0 to 0.6. The density of pure liquids and liquid mixtures were determined using a pycnometer and gave an estimated reproducibility of $\pm 0.0001 \text{ g cm}^{-3}$. The ultrasonic velocity was measured by using an ultrasonic interferometer (Model: F81) supplied by M/S Mittal Enterprises, New Delhi, having the frequency 3 MHz with an overall accuracy of $\pm 0.1 \text{ ms}^{-1}$.

Theory

Experimentally measured ultrasonic velocity has been compared with those obtained from the following equations⁷⁻¹⁰;

Nomoto's relation (NR)

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

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.

$$\text{Where molar sound velocity } R = \frac{M}{\rho} U^{1/3} = V U^{1/3}$$

$$\text{The molar volume } V = \frac{M}{\rho}$$

Ideal mixture relation (IMR)

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

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

$$\alpha = \left(\frac{U^2 \exp}{U_{IMR}^2} \right) - 1 \quad (3)$$

Impedance dependence relation (IDR)

$$U_{IDR} = \frac{\sum_{i=1}^3 X_i Z_i}{\sum_{i=1}^3 X_i \bar{n}_i} \quad (4)$$

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

Collision factor theory (CFT)

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

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

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

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

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 Avagadro Number

Percentage deviation

The percentage deviation 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 velocity and the estimated ultrasonic velocity from the various theoretical models for three systems are summarized in the Table 1. The limitations and approximations incorporated in these theories are responsible for it.

Table 1. Values of experimental, 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 I-Propanol +Toluene + Dibutylether						
0.0000	0.6000	1181.9	1180.9	1185.4	1200.4	1195.8
0.0999	0.5000	1185.9	1186.3	1169.4	1204.9	1195.4
0.2000	0.4000	1190.0	1192.5	1160.1	1209.3	1201.3
0.3000	0.3000	1197.7	1199.7	1157.6	1213.8	1206.0
0.4000	0.2000	1204.4	1208.4	1161.4	1218.1	1210.1
0.5000	0.1000	1217.2	1218.7	1171.7	1222.5	1214.8
0.6000	0.0000	1225.7	1231.4	1189.3	1226.9	1216.1
System II-Butanol +Toluene + Dibutylether						
0.0000	0.6000	1181.9	1180.9	1185.4	1200.4	1195.8
0.1000	0.5000	1186.4	1188.4	1185.7	1208.1	1202.2
0.2000	0.4000	1196.4	1197.0	1189.0	1215.7	1211.7
0.3000	0.3000	1200.7	1206.6	1195.3	1223.3	1217.4
0.4000	0.2000	1211.8	1217.7	1204.8	1230.7	1226.7
0.5000	0.1000	1222.9	1230.5	1217.6	1238.1	1234.5
0.6000	0.0000	1236.6	1245.5	1234.1	1245.4	1240.0
System III-Pentanol+Toluene + Dibutylether						
0.0000	0.6000	1181.9	1180.9	1185.4	1200.4	1195.8
0.1001	0.5000	1191.2	1191.3	1194.8	1211.3	1207.3
0.2000	0.4001	1202.6	1202.8	1205.7	1222.1	1221.2
0.3000	0.3000	1216.7	1215.4	1217.9	1232.8	1232.0
0.4000	0.2000	1228.1	1229.5	1231.4	1243.4	1242.0
0.5000	0.1000	1247.0	1231.6	1121.1	1244.5	1379.1
0.6000	0.0000	1255.3	1262.9	1263.3	1264.2	1261.2

It is assumed that all the molecules are spherical in shape, which is not true every time. According to Nomoto's theory, it is assumed that the volume does not change on mixing. Therefore, no interaction between the components of liquid mixtures has been taken into account. Similarly, the assumption for the formation of ideal mixing relation is that, the ratios of specific heats of ideal mixtures and the volumes are also equal. Again, no molecular interaction is taken into account. But on mixing two liquids, the interaction takes place because of various forces such as dispersion forces, charge transfer, hydrogen bonding, dipole-dipole and dipole-induced dipole interactions. Thus the observed deviation of theoretical values of velocity from the experimental values shows that the molecular interaction is taking place between the unlike molecules in the liquid mixture⁴.

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}
System I-Propanol +Toluene + Dibutylether				
	0.09	0.29	1.56	1.18
	0.12	1.31	1.69	0.89
	0.21	2.51	1.63	0.96
	0.17	3.34	1.34	0.69
	0.33	3.57	1.15	0.48
	0.13	3.73	0.44	0.20
	0.47	2.96	0.09	0.78
APE	0.22	2.53	1.13	0.74
SPE	0.25	2.79	1.27	0.80
System II-Butanol +Toluene + Dibutylether				
	0.08	0.28	1.56	1.19
	0.17	0.06	1.83	1.33
	0.05	0.62	1.61	1.28
	0.50	0.45	1.88	1.39
	0.49	0.58	1.56	1.23
	0.62	0.43	1.24	0.95
	0.72	0.20	0.71	0.28
APE	0.38	0.37	1.48	0.89
SPE	0.45	0.42	1.53	1.15
System III-Pentanol+Toluene + Dibutylether				
	0.08	0.28	1.56	1.19
	0.01	0.31	1.69	1.35
	0.01	0.25	1.62	1.54
	0.11	0.10	1.33	1.26
	0.11	0.27	1.25	1.13
	1.24	10.1	0.20	10.6
	0.60	0.63	0.71	0.47
APE	0.31	1.71	1.19	2.51
SPE	0.52	3.83	1.30	4.16

1- Propanol + Toluene + Dibutylether

From the Table 2, it is evident that the ultrasonic velocities calculated by Nomoto's relation deviate from 0.09 to 0.47%, IMR shows a deviation of 0.29 to 3.73%, IDR deviate by 0.09

to 1.69% and finally CFT makes a deviation of 0.2 to 1.18 over the entire concentration of 1-propanol. It is observed from the values of APE & SPE (Table 2), the results for 1-propanol system in the order of NR, CFT, IDR and IMR.

1-Butanol + Toluene + Dibutylether

Table 2 shows, the deviation for the ultrasonic velocities calculated by NR, IMR, IDR and CFT in the range of 0.05 to 0.72% 0.06 to 0.62%, 0.71 to 1.88% and 0.28 to 1.39% respectively. From Table 2, it is evident that the theories agree well with the experimental values in the order of IMR, NR, CFT and IDR.

1-Pentanol + Toluene + Dibutylether

The value of percentage deviation (Table 2) for system III using NR is in the range of 0.01 to 1.24%, IMR in the range of 0.10 to 10.1%, then the IDR is of 0.20 to 1.69% and finally CFT is of 0.47 to 10.6%. From the above results it is observed that the theories in the order of NR, IDR, IMR and CFT.

Conclusion

Ultrasonic velocities predicted using NR, IMR, IDR and CFT were compared with experimentally measured velocity values at 303K in the three component mixtures of dibutylether and toluene with *n*-alkanols. Among the four theories, it is found that the NR is in best suited with the experimental velocity values.

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