

Impact of Intermolecular Interaction In Binary Blends From Estimated Sound Velocity

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Abstract

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Purpose: To understand the nature of liquids the need of physico-chemical behavior of liquid mixtures or in pure form Sound velocity, viscosity and density values have been calibrated in binary and ternary system of some of the Aniline+1-alkanols with benzene, toluene, and hexane at 303K. Several theoretical models have been applied to evaluate the sound velocity values for the binary and ternary systems compared with the experimental values.

Method: The ultrasonic velocity, density and viscosity measured with ultrasonic interferometer, specific gravity bottle with Oswald's viscometer respectively. The measured ultrasonic velocity compared with theoretical models to understand the existence of molecular interactions from models like Nomoto' Relation, Free Length Theory, ideals mixture relation etc.

Results: NR predictions provide better closeness with test values and FLT predictions are not completely acceptable. FLT prediction is found to fail even for pure liquids. IMR predictions are more acceptable than NR, only for aniline + 1-pentanol binary and NR seem to be the best of all other systems. In binary, IMR predicted values are always lower than test values, but NR predictions are, in most cases, higher than test values. In ternary systems, especially at high mole fractions of aniline, the predicted sound velocity values (NR & IMR) are always lower than the experimentally observed values. Among the many theories considered, NR gives the best prediction of sound speed. The sequence of qualifications for predicting sound speed decreases as NR and IMR and FLT are completely invalid for all considered systems.

Conclusion: Strong molecular interaction with the structure formation increases with mole fractions. Azeotropic destruction has been found to be the most common of the compounds considered.

Keywords: Binary blend, Molecular interaction, Estimated sound velocity, statistical model.

Introduction

Sound velocity estimates can also be used to estimate the nature of molecular reactions in liquid compounds. The disappearance from linearity in the values of ultrasound velocity when studied as a function of concentration is found to exhibit



interesting variations in the case of liquid mixtures (Pandey & Shukla, 1977; Khanwalkar, 1989; Pandey et al., 1989; Oswal et al., 1998). The estimated acoustic and thermodynamic properties of the binary and ternary fluid compounds reported in the previous documents (Palaniappan, 2001; Palaniappan et al., 2020; Kannappan & Palaniappan, 1999; IUPAC, 1995) represent the physico-chemical and molecular interactions between the components of the system.

As an additional confirmation of the existence of a specific interaction, this work attempts to show a relationship of experimental findings of sound speed with those theoretically predicted based on molecular models. Such comparisons are useful in understanding the thermodynamics of compounds and provide the best means to test the validity of many empirical and semi-empirical theories (McMurry, 2007; Kannappan & Palaniappan, 1999b).

In recent years, various theories (Sadasiva Rao et al., 2000; Dean, 1987; Ali et al., 2003; Sasikumar et al., 2015a) have been used to calculate the ultrasonic velocity in liquid mixtures, and the difference in theoretical sound velocity has been recognized mainly for molecular interactions in compounds. In this work, the theoretical evaluation of ultrasonic velocity in the binary and ternary liquid mixtures studied in binary and ternary liquids blend have been done using Nomoto's relation, Van Deal Vangeal's ideal mixture relation and Free length theory (Palaniappan, 2001; Palaniappan et al., 2020; Kannappan & Palaniappan, 1999; IUPAC, 1995; McMurry, 2007; Kannappan & Palaniappan, 1999b; SadasivaRao et al., 2000; Dean, 1987; Ali et al., 2003; Sasikumar et al., 2015a; Nomoto, 1958; Van Deal & Vangeal, 1969; Jacobson et al., 1952; Jacobson, 1951, Palaniappan, 1998; Pearson, 1978). Also, percentage deviation, molecular interaction parameter and Chi-square test values are calculated. These statistical parameters support the predictions made and verify the validity of the theory for the observational methods.

Experimental details

The liquid combinations of various concentrations in mole fraction were prepared by taking AR grade chemicals, which were decontaminate by standard methods (Rowlinson, 1959). The ultrasonic velocity (U) in liquid blends have been deliberated using an ultrasonic interferometer (Mittal type ,Model F-80) working at 2 MHz frequency with an accuracy of $\pm 0.1 \text{ ms}^{-1}$. The density (ρ) and viscosity(η) are deliberated using a pycknometer and an Ostwald's viscometer respectively with an accuracy of 3 parts in 105 for density and 0.001 Nsm⁻² for viscosity.

Using the deliberated data, the phonic restrictions such as adiabatic compressibility(β_a), free length(Lf), free volume(Vf), and internal pressure(π_i) and their surplus restrictions have been enumerated using the standard expressions (Kannappan et al., 1991; Sasikumar et al., 2015b).

Theory and Calculations

1. Nomoto's Relation [NR]

Nomoto (15) established an empirical formula for ultrasonic velocity in binary liquid mixtures on the hypothesis of linear dependence of the molar sound velocity on concentration in mole fraction and the additive for molar volume as,

$$U = \left(\frac{x_1 R_1 + x_2 R_2}{X_1 V_1 + x_2 V_2} \right)^3 \quad (1)$$

Where, x_1, x_2 are the mole fraction of the components. R_1, R_2 the respective molar sound velocities and V_1, V_2 the molar volumes respectively.

Molar sound velocity is related to molecular weight [m] and density [ρ] as,

$$R = \frac{m}{\rho} U^{3/2} = V U^{3/2} \quad (2)$$

Where, the molar volume obeys the additive property

$$V = x_1 V_1 + x_2 V_2 + x_3 V_3 \quad (3)$$

2. Ideal Mixture Relation [IMR]

Van deal and Vangeal (Van Deal & Vangeal, 1969) assumed the adiabatic compressibility (β) of the mixture as on the basis of ideal behaviour, the sound velocity is given as,

$$\frac{1}{(x_1 m_1 + x_2 m_2) U_{IMR}^2} = \frac{X_1}{m_1 U_1^2} + \frac{X_2}{m_2 U_2^2} \quad (4)$$

The degree of molecular interaction α is given as,

$$\alpha = \left[\frac{U_{\text{expt}}^2}{U_{IMR}^2} \right] - 1 \quad (5)$$

3. Free Length Theory [FLT]

Jacobson (Jacobson et al., 1952; Jacobson, 1954) introduced the concept of interpolation free length to determine the ultrasonic velocity in pure liquids and liquid mixtures. Furthermore, he correlated the velocity of pure fluids with the free length LF,

$$U L_f \rho^{1/2} = K_T \quad (6)$$

where, K_T is the temperature dependent Jacobson's constant which takes a value of 199.976×10^{-8} in M.K.S. units at 303 K. For liquid mixtures, the above equation can be written as,

$$U_{FLT} = \frac{K_T}{L_{\text{mix}} \rho^{1/2}} \quad (7)$$

where, L_{mix} and ρ represents the free length and density of the mixture.

4. Percentage Deviation

Percentage deviation in sound speed between experimental and computed values is calculated (Pandey & Shukla, 1977),

$$\left[\frac{\Delta U}{U} \right] \% = \left[\frac{U_{\text{expt}} - U_{\text{the}}}{U_{\text{expt}}} \right] \cdot 100\% \quad (8)$$

5. Chi-Square Test for Goodness of Fit

Karl Pearson (Palaniappan, 1998; Pearson, 1978) Benefit testing is a very powerful tool for determining whether deviations from theoretical values from test subjects are likely due to a lack of applicability theory in the data.. If O_i [$i=1,2,3 \dots n$] is a set of observed frequencies and E_i [$i=1,2,3 \dots n$] is the corresponding set of theoretical frequencies, then the Chi-square is given by,

$$(\chi)^2 = \sum_{i=1}^n \left[\frac{(O_i - E_i)^2}{E_i} \right] \quad (9)$$

For the best correlation, the calculated χ^2 should be less than 1.239 for 1 % error.

Results and Discussions

The experimentally measured ultrasonic velocity values and the estimated ultrasonic velocities obtained from several theoretical models for the binary and ternary systems taken in this study are given in Tables 1. The percentage deviation of the ultrasonic velocity, the molecular interaction parameter (∞) and the Chi-square deviation of the theoretical velocities from the experimental values for the respective systems are given in the same table. (Fig .1(a-d) shows the trend of molecular interaction parameter for all the four binary systems.

Table 1. Estimated Sound Velocities and their Validation Parameters for Benzene, Toluene, Hexane and Aniline Binaries

Mole fraction		Ultrasonic velocity in ms ⁻¹				Percentage deviation of velocity			α	Ultrasonic velocity in ms ⁻¹				Percentage deviation of velocity			α	
x_1	x_3	U_{expt}	U_{NR}	U_{IMR}	U_{FLT}	U_{NR}	U_{IMR}	U_{FLT}		U_{expt}	U_{NR}	U_{IMR}	U_{FLT}	U_{NR}	U_{IMR}	U_{FLT}		
Benzene Binaries																		
1-PENTANOL SYSTEM									1-HEXANOL SYSTEM									
0.0	1.0	1251.1	1253.1	1253.6	1198.1	0.000	0.000	4.867	0.000	1261.1	1261.1	1261.1	1211.0	0.000	0.000	3.948	0.000	
0.1	0.9	1268.3	1273.0	1259.0	1208.3	-0.370	-0.055	4.730	0.001	1282.5	1286.3	1273.0	1226.3	-0.296	0.740	4.382	0.014	
0.2	0.8	1273.5	1286.3	1268.1	1226.0	-1.009	-0.362	3.729	0.019	1289.6	1294.2	1286.7	1244.4	-0.356	0.224	3.497	0.012	
0.3	0.7	1288.0	1297.2	1272.3	1240.6	-0.714	-0.333	3.680	0.014	1298.1	1301.0	1289.9	1265.0	-0.246	0.631	2.549	0.022	
0.4	0.6	1295.6	1310.2	1289.0	1254.7	-1.126	0.509	3.156	0.022	1301.4	1308.1	1289.4	1282.1	-0.514	0.230	1.483	0.046	
0.5	0.5	1305.6	1322.0	1297.0	1268.2	-2.509	0.608	2.798	0.031	1312.0	1316.3	1309.0	1295.6	-0.327	0.228	1.280	0.045	
0.6	0.4	1315.0	1383.7	1312.4	1285.0	-1.802	0.197	2.281	0.037	1325.3	1329.6	1319.6	1309.8	-0.324	0.430	1.169	0.036	
0.7	0.3	1324.2	1350.6	1319.2	1304.1	-1.392	1.735	2.860	0.029	1331.3	1338.0	1327.2	1324.9	-0.503	0.307	0.480	0.026	
0.8	0.2	1342.5	1361.2	1336.0	1323.6	-1.392	0.484	1.407	0.022	1350.3	1359.4	1345.4	1337.5	-0.673	0.362	0.947	0.017	
0.9	0.1	1366.0	1370.0	1358.2	1345.2	-2.940	1.407	0.522	0.002	1368.0	1370.5	1362.1	1358.7	-0.182	0.431	0.679	0.008	
1.0	0.0	1377.3	1377.3	1377.3	1384.0	0.000	0.000	-0.486	0.000	1377.3	1377.3	1377.3	1384.0	0.000	0.000	-0.486	0.000	
Chi-square values						$(\chi)^2$	0.034	1.083	21.091	-					0.041	0.639	17.421	-
1-HEPTANOL SYSTEM																		
0.0	1.0	1222.0	1222.0	1222.0	1198.7	0.000	0.000	1.906	0.000									
0.1	0.9	1298.0	1299.9	1289.1	1216.9	-0.146	0.685	6.248	0.002									
0.2	0.8	1306.3	1308.2	1299.6	1237.3	-0.145	0.512	5.282	0.013									
0.3	0.7	1318.1	1321.4	1308.3	1256.1	-0.250	0.743	4.665	0.015									
0.4	0.6	1332.5	1338.6	1326.1	1277.9	-0.457	0.480	4.097	0.019									
0.5	0.5	1346.0	1350.0	1338.0	1295.8	-0.297	0.594	3.729	0.029									
0.6	0.4	1358.5	1362.3	1342.6	1317.7	-0.279	1.170	3.003	0.023									
0.7	0.3	1368.6	1369.7	1356.8	1336.3	-0.018	0.862	2.360	0.017									
0.8	0.2	1370.2	1372.4	1364.0	1336.0	-0.160	0.452	2.495	0.009									
0.9	0.1	1375.0	1376.2	1371.2	1363.2	-0.160	0.276	0.858	0.005									
1.0	0.0	1377.3	1377.3	1377.3	1384.0	0.000	0.000	-0.486	0.000									
Chi-square values						$(\chi)^2$	0.028	0.936	24.562	-								
Toluene Binaries																		
1-PENTANOL SYSTEM									1-HEXANOL SYSTEM									
0.0	1.0	1253.2	1253.2	1253.2	1231.6	0.000	0.000	1.7235	0.000	1261.1	1261.1	1261.1	1211.0	0.000	0.000	3.924	0.000	
0.1	0.9	1210.3	1215.0	1208.0	1240.9	-0.388	0.198	-2.528	0.003	1278.3	1281.4	1275.6	1222.2	-0.242	0.211	4.388	0.004	
0.2	0.8	1223.4	1226.2	1219.7	1249.1	-0.228	0.302	-2.100	0.006	1284.6	1287.0	1280.0	1233.5	-0.186	0.358	3.977	0.007	
0.3	0.7	1228.6	1239.1	1222.0	1258.7	-0.834	0.537	-2.449	0.010	1293.2	1293.2	1287.3	1244.3	-0.224	0.232	3.565	0.014	
0.4	0.6	1232.5	1236.4	1230.3	1266.5	-0.316	0.178	-2.310	0.018	1294.2	1296.4	1290.4	1254.1	-0.919	0.293	3.098	0.025	
0.5	0.5	1246.7	1248.1	1239.6	1275.5	-0.112	0.569	-2.310	0.018	1296.4	1301.1	1293.6	1264.8	-0.377	0.215	2.437	0.043	
0.6	0.4	1250.2	1253.4	1248.3	1283.7	-0.255	0.151	-2.679	0.023	1301.2	1306.9	1299.9	1275.8	-0.438	0.099	1.952	0.022	

0.7	0.3	1263.0	1266.0	1257.8	1292.8	-0.237	0.411	-2.359	0.017	1310.4	1313.4	1306.4	1285.4	-0.228	0.305	1.907	0.016
0.8	0.2	1272.4	1278.2	1268.4	1301.0	-0.455	0.314	-2.357	0.006	1318.4	1321.0	1312.3	1295.0	-0.197	0.462	1.774	0.009
0.9	0.1	1281.6	1284.6	1278.1	1310.1	-0.234	0.273	-2.223	0.005	1322.6	1328.6	1319.4	1306.3	-0.453	0.241	1.232	0.004
1.0	0.0	1287.2	1287.2	1287.2	1318.9	0.000	0.000	-2.430	0.000	1287.6	1287.6	1287.6	1318.9	0.000	0.000	-2.430	0.000
Chi-square values					(χ) ²	0.033	0.492	31.043	-					0.049	0.384	16.5480	-

1-HEPTANOL SYSTEM

0.0	1.0	1222.0	1222.0	1222.0	1198.7	0.000	0.000	1.906	0.000
0.1	0.9	1227.3	1229.1	1220.3	1211.9	-0.146	0.570	1.254	0.011
0.2	0.8	1233.6	1236.4	1226.2	1223.7	-0.226	0.599	0.802	0.012
0.3	0.7	1239.4	1242.0	1234.0	1236.9	-0.209	0.435	0.201	0.017
0.4	0.6	1244.2	1248.6	1241.6	1249.7	-0.353	0.208	-0.442	0.024
0.5	0.5	1251.1	1253.7	1248.4	1262.5	-0.207	0.215	-0.911	0.018
0.6	0.4	1257.6	1260.3	1252.1	1275.0	-0.214	0.437	-1.383	0.015
0.7	0.3	1262.2	1265.9	1259.0	1288.3	-0.293	0.253	-2.067	0.012
0.8	0.2	1270.0	1273.0	1268.3	1301.3	-0.236	0.133	-2.464	0.008
0.9	0.1	1280.3	1282.1	1268.3	1313.8	-0.140	0.133	-2.616	0.005
1.0	0.0	1287.6	1287.6	1287.6	1318.9	0.000	0.000	-2.430	0.000
Chi-square values					(χ) ²	0.034	0.401	11.845	-

Hexane Binaries**1-PENTANOL SYSTEM****1-HEXANOL SYSTEM**

0.0	1.0	1253.0	1253.0	1253.0	1231.6	0.000	0.000	1.707	0.000	1261.1	1261.1	1261.1	1211.0	0.000	0.000	3.972	0.000
0.1	0.9	1259.6	1261.7	1247.2	1249.4	-0.166	0.984	0.809	0.009	1276.0	1280.2	1269.9	1231.7	-0.329	0.478	3.471	0.005
0.2	0.8	1265.4	1269.4	1255.1	1266.7	-0.316	0.813	-0.102	0.012	1284.3	1287.0	1278.2	1251.8	-0.210	0.474	2.530	0.009
0.3	0.7	1272.2	1278.0	1263.9	1285.0	-0.455	0.652	-1.006	0.013	1289.6	1292.3	1281.4	1271.1	-0.209	0.635	1.434	0.012
0.4	0.6	1277.0	1282.1	1267.6	1303.3	-0.399	0.736	-2.059	0.014	1296.0	1299.6	1292.0	1294.9	-0.277	0.308	0.108	0.018
0.5	0.5	1285.4	1290.3	1279.1	1319.7	-0.381	0.490	-2.668	0.017	1302	1308.5	1397.1	1314.9	-0.290	0.382	-1.972	0.017
0.6	0.4	1294.6	1296.9	1289.3	1337.9	-0.177	0.409	-3.344	0.019	1308.2	1312.0	1303.2	1334.0	-0.290	0.382	-1.972	0.017
0.7	0.3	1301.0	1309.4	1292.2	1354.2	-0.645	0.676	-4.089	0.014	1315.6	1319.4	1310.3	1352.2	-0.288	0.402	-2.782	0.008
0.8	0.2	1307.1	1312.6	1297.8	1370.4	-0.420	0.711	-4.842	0.012	1322.5	1327.3	1318.6	1369.0	-0.363	0.295	-3.517	0.005
0.9	0.1	1315.1	1317.9	1308.9	1388.7	-0.144	0.471	-5.596	0.006	1332.0	1340.1	1327.2	1388.7	-0.608	0.360	-4.256	0.003
1.0	0.0	1158.4	1158.4	1158.4	1398.2	0.000	0.000	-20.074	0.000	1158.4	1158.4	1158.4	1398.2	0.000	0.000	-20.074	0.000
Chi-square values					(χ) ²	0.036	0.542	20.125	-					0.054	0.482	15.632	-

1-HEPTANOL SYSTEM

0.0	1.0	1222.0	1222.0	1222.0	1198.7	0.000	0.000	1.906	0.000
0.1	0.9	1228.1	1232.6	1223.5	1221.8	-0.366	0.374	0.512	0.007
0.2	0.8	1237.6	1242.1	1234.6	1244.0	-0.363	0.282	-0.517	0.012
0.3	0.7	1245.0	1248.8	1241.1	1267.1	-0.305	0.313	-1.775	0.016
0.4	0.6	1252.4	1256.2	1248.8	1289.3	-0.303	0.388	-2.946	0.022
0.5	0.5	1260.7	1265.5	1255.8	1310.6	-0.267	0.654	-4.807	0.031
0.6	0.4	1268.9	1272.3	1260.6	1329.9	-0.267	0.654	-4.807	0.023
0.7	0.3	1275.4	1280.2	1272.6	1354.2	-0.376	0.219	-5.178	0.014
0.8	0.2	1284.6	1286.9	1281.3	1375.5	-0.179	0.256	-6.076	0.008
0.9	0.1	1296.3	1298.6	1292.0	1383.0	-0.177	0.331	-7.688	0.006
1.0	0.0	1158.4	1158.4	1158.4	1398.2	0.000	0.000	-20.700	0.000
Chi-square values					(χ) ²	0.037	0.432	14.036	-

Aniline Binaries

1-PENTANOL SYSTEM

1-HEXANOL SYSTEM

0.0	1.0	1253.1	1253.1	1253.1	1231.6	0.000	0.000	1.715	0.000	1261.1	1261.1	1261.1	1211.0	0.000	0.000	3.972	0.000	
0.1	0.9	1347.0	1357.2	1328.0	1273.4	-0.757	1.410	5.463	0.008	1285.0	1294.2	1273.4	1257.6	-0.715	0.902	2.132	0.008	
0.2	0.8	1358.1	1364.2	1346.9	1314.0	-0.449	0.824	3.247	0.016	1344.5	1354.7	1337.5	1303.9	-0.758	0.520	3.019	0.012	
0.3	0.7	1401.0	1408.9	1387.2	1258.5	-0.563	0.985	3.033	0.019	1353.0	1358.5	1346.1	1352.0	-0.406	0.509	0.073	0.019	
0.4	0.6	1429.3	1435.6	1418.7	1408.1	-0.440	0.741	1.483	0.024	1357.0	1361.3	1349.5	1401.4	-0.316	0.552	-3.271	0.021	
0.5	0.5	1494.4	1505.2	1486.3	1456.8	-0.722	0.569	2.516	0.027	1384.5	1390.3	1377.9	1447.6	-0.418	0.476	-4.557	0.029	
0.6	0.4	1510.0	1525.6	1501.4	1506.2	-0.033	0.569	0.251	0.019	1442.0	1447.9	1434.1	1496.3	-0.409	0.547	-3.765	0.021	
0.7	0.3	1554.2	1564.3	1526.7	1561.6	-0.649	1.769	-0.476	0.016	1473.3	1480.6	1463.6	1521.0	-0.495	0.658	-3.237	0.012	
0.8	0.2	1594.6	1599.4	1572.1	1699.3	-0.301	1.411	-0.189	0.018	1532.4	1538.2	1523.8	1563.1	-0.378	0.561	-2.003	0.011	
0.9	0.1	1612.0	1624.0	1598.7	1601.0	-0.744	0.825	-0.652	0.016	1559.0	1550.4	1543.0	1592.3	-0.251	1.026	-2.135	0.006	
1.0	0.0	1614.3	1614.3	1614.3	1618.3	0.000	0.000	-0.247	0.000	1614.3	1614.3	1614.3	1618.3	0.000	0.000	-0.247	0.000	
Chi-square values						(χ) ²	1.623	1.489	15.053	-					0.259	0.612	11.042	-

1-HEPTANOL SYSTEM

0.0	1.0	1222.0	1222.0	1222.0	1198.7	0.000	0.000	1.906	0.000	
0.1	0.9	1228.1	1232.6	1223.5	1221.8	-0.366	0.374	0.512	0.007	
0.2	0.8	1237.6	1242.1	1234.6	1244.0	-0.363	0.282	-0.517	0.012	
0.3	0.7	1245.0	1248.8	1241.1	1267.1	-0.305	0.313	-1.775	0.016	
0.4	0.6	1252.4	1256.2	1248.8	1289.3	-0.303	0.388	-2.946	0.022	
0.5	0.5	1260.7	1265.5	1255.8	1310.6	-0.267	0.654	-4.807	0.031	
0.6	0.4	1268.9	1272.3	1260.6	1329.9	-0.267	0.654	-4.807	0.023	
0.7	0.3	1275.4	1280.2	1272.6	1354.2	-0.376	0.219	-5.178	0.014	
0.8	0.2	1284.6	1286.9	1281.3	1375.5	-0.179	0.256	-6.076	0.008	
0.9	0.1	1296.3	1298.6	1292.0	1383.0	-0.177	0.331	-7.688	0.006	
1.0	0.0	1158.4	1158.4	1158.4	1398.2	0.000	0.000	-20.700	0.000	
Chi-square values						(χ) ²	1.698	1.823	28.512	-

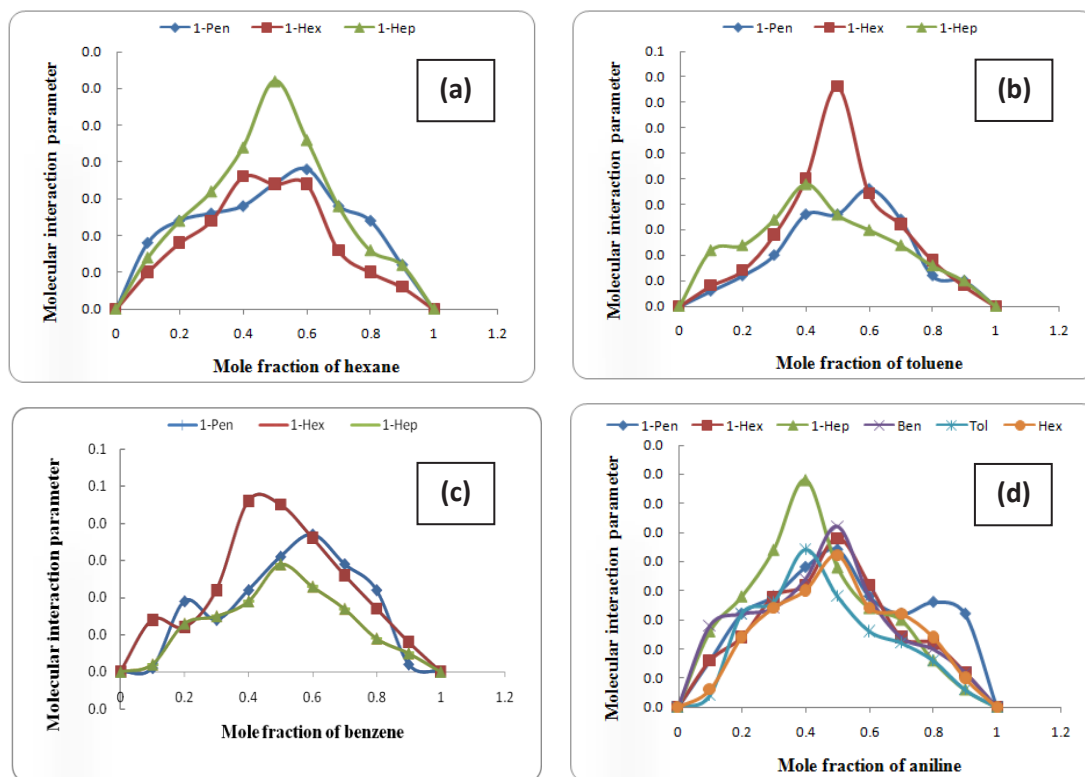


Figure 1. Trend of Molecular Interaction Parameter in (a) benzene, (b) toluene, (c) hexane and (d) aniline binaries

The study of Table 1 reveals the good and bad agreement between the observed and calculated sound speeds, due to the many assumptions and approximations made in the respective theories. It can be observed that in all systems of binaries, NR predictions provide better closeness with test values and FLT predictions are not completely acceptable. FLT prediction is found to fail even for pure liquids. IMR predictions are more acceptable than NR, only for aniline + 1-pentanol binary and NR seem to be the best of all other systems. In binary, IMR predicted values are always lower than test values, but NR predictions are, in most cases, higher than test values.

Among the many theories considered, NR gives the best prediction of sound speed. The sequence of qualifications for predicting sound speed decreases as NR and IMR and FLT are completely invalid for all considered systems.

Discussions on Percentage Deviations

The average percentage deviations between the observed and calculated sound velocities may be due to molecular interactions between the components of the liquid mixture (SadasivaRao et al., 2000; Ali et al., 2003; Sasikumar et al., 2015a; Nomoto, 1958). Such types of interactions are not considered in the practice of the respective theories. Furthermore, in many ultrasonic processes they are not sufficient to compute in detail the experimental expression of molecular interactions. The magnitude of the deviation in velocities may be due to the assumptions made in the theories of weak polar interactions between polar-polar and polar-molecules.

Discussions on Molecular Interaction Parameter

The molecular contact parameter, which is given as the deviation of the value of U_{2exp} / U_{2IMR} from the uniformity, is an effective verification parameter that confirms the size of the interactions between the components of the compound and determines whether the selected compound is optimal or not. These values are also presented in the same Table.1 and clearly plotted in fig.1(a-d). It is capable of specifying the number of molecular interactions in liquid compounds, especially in other cases where the speed of sound is unknown.

Verification arises from Chi-square deviations. The predictions based on percentage deviation and Chi-square test can be seen to be similar, although the predictions of the Chi-square test are clear. The Chi-square test of fit advantage helps to determine whether the possibility of deviation of theoretical values from the test subjects is due to the inadequacy of the applicable theory in the data.

Discussions on Chi-Square Deviations

Chi-square follows Chi-square distribution with $(n-1)$ degrees of freedom. For a set of eleven readings of the present investigations for binary mixtures, it is noted that if the χ^2 value is less than 2.558, the theoretical values are acceptable as having only 1% error. To accept 5% error, χ^2 values may go up to 3.940. Chi-square values for different theoretical methods are presented in same Table.1.

Validations of Theoretical Comparison

Table.1 also relate binary compounds to second components containing 1-alkanols (polarization), while weak polarization in the first three systems (ie benzene, toluene and hexane) and strong polar (aniline) in the first three systems, A perusal of these Table.1 reveals that the percentage deviation for NR is comparatively lower than that for IMR whereas they are totally invalid for FLT.

FLT method assumes that the molecules are behaving as rigid spheres (Pearson, 1978; Rowlinson, 1959). Therefore, the hardness of the components cannot be calculated due to the failure of the FLT, and the component appears to be more elastic and flexible. This flexibility system is expected to be even more efficient.

For a better combination, the IMR predictions should match the experimental values. This is also inferior in current systems as IMR predictions have only a second qualification, so the systems are unrealistic. This loss in elasticity may be attributed to the fact that the components are involving in azeotropic / complex formation. Thus, the estimation of sound speed supports the scenarios obtained in all binary systems in this view. As suggested from the relative instability of the measured area of binary compounds, these scenarios provide the necessary validation for non-conceptualization of systems (Palaniappan, 1998; Palaniappan & Nithiyantham, 2019).

From these tables it can be seen that NR fits unanimously, while FLT does not apply to polar-polar type (aniline + alcohol systems) and nearby best combinations. Since the linear dependence of the speed of sound on the mole fraction is essentially based on Nomoto's method, the increasing mole fraction increases the existing structure in the system, thus, the increase of the first components supports the regular structure-formation. This view of the experimental part (Sasikumar et al., 2015b; Hykes et al., 1983; C. Reddy et al., 1964; Palaniappan et al., 2020).

Furthermore, for NR predictions, % deviations from benzene, toluene, and hexane binary are often negative and low. However, for some aniline binary they are positive and higher than IMR predictions. NR method demands the dependence of molar sound velocity and hence this may be obviously true for the chosen binaries (Palaniappan et al., 2020). The smallest magnitudes of % deviation express closeness with experimental values, so it is clear that molar sound velocity plays an important role in determining molecular interactions.

The molecular interaction parameter α is small but positive in all the mixtures. This observed α values clearly indicate the existence of strong interactions existing between the polar-polar and polar – weak-polar molecules. The percentage deviation and C-square values obtained for IMR are very high FLT. This is completely unclear, indicating that these theories are invalid

The system is considered. This is also reflected in the large percentage deviation of sound speed. Theoretical study further confirms that there are strong interactions between the component molecules in the compounds that arise due to the disruption of the molecular symmetry of the polar molecules, as similar explanations have been made for the current structure (Sivanarayana et al., 1982; Tiwari et al., 1995; Bhatti & Singh, 1983; Mishra & Pandey, 1979; Ramaswamy et al., 1980; Palaniappan & Nithiyantham, 2019).

Recommendations for the use of IMR are not considered final, as the IMR system is a complete failure. They need to be further refined. This can be done with the obtained C square values. As mentioned earlier, a c square equal to or less than 2.558 for binary indicates a 1% error in the prediction, which can be up to 3.940 for a 5% error. Therefore, all binary systems except aniline + hexane fully meet the NR assumptions. Thus, the dependence of the sound velocity on the mole fraction is detected. System Aniline + Hexane seem to be the best (Palaniappan et al., 2003; Palaniappan et al., 2020b; Palaniappan et al., 2020).

Table.1 further indicates that the amount of contact with the chain structural degenerates increases, i.e., the maximum contact is for 1-pentanol and the minimum for 1-heptanol. Maximum contact with 1-pentanol system is observed. The chances of azeotropic / complex destruction of aniline binary complexes is much higher in the benzene and toluene systems than in the hexane systems (Sasikumar et al., 2018; de Oliveira et al., 2020; Palaniappan & Nithiyantham, 2019). Furthermore, these differences confirm the dependence of the chain length on the molecular contact.

Conclusion

The above discussion leads to the following conclusions:

1. Of the three theories taken for the prediction of sound speed, NR will give the best comparison with the test value for the systems investigated. The existence of strong interactions between the components of the mixture is evident.
2. Components of the systems, especially in ternary, are found to be not rigid, non-ideal and depend on molar sound velocity.
3. Increasing the mole fraction increases the structure formation in all systems.
4. Azeotropic destruction has been found to be the most common of the compounds considered

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تأثير التفاعل بين الجزيئات في التوليفات الثنائية من سرعة الصوت المقدر

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المستخلص

الهدف: لفهم طبيعة السوائل، فإن الحاجة إلى السلوك الفيزيائي والكيميائي للمخاليط السائلة أو في صورة نقية تمت معايرة قيم سرعة الصوت والزوجة والكثافة في النظام الثنائي والثلاثي لبعض من الأنيلين + -1 الكانول مع البنزين والتولوين والهكسان عند 303 ألف. تم تطبيق العديد من النماذج النظرية لتقييم قيم سرعة الصوت للنظام الثنائي والثلاثي مقارنة بالقيم التجريبية.

الطريقة: يتم قياس السرعة والكثافة والزوجة بالموجات فوق الصوتية باستخدام مقياس التداخل بالموجات فوق الصوتية، وزجاجة الجاذبية النوعية بمقياس الزوجة من أوزوالد على التوالي. السرعة بالموجات فوق الصوتية المقاسة مقارنة بالنماذج النظرية لفهم وجود التفاعلات الجزيئية من نماذج مثل علاقة نوموتو ونظرية الطول الحر وعلاقة المزيغ المثالية وما إلى ذلك.

النتائج: توفر تنبؤات NR تقاربًا أفضل مع قيم الاختبار وتنبؤات FLT غير مقبولة تمامًا. تم العثور على تنبؤ FLT فشل حتى بالنسبة للسوائل النقية. تنبؤات IMR مقبولة أكثر من NR، فقط للأنيلين + -1 بنتانول ثنائي ويبدو أن NR هو الأفضل من بين جميع الأنظمة الأخرى. في النظام الثنائي، تكون القيم المتوقعة لـ IMR دائمًا أقل من قيم الاختبار، ولكن تنبؤات NR، في معظم الحالات، أعلى من قيم الاختبار. في الأنظمة الثلاثية، خاصة في الأجزاء المولية العالية من الأنيلين، تكون قيم سرعة الصوت المتوقعة (NR & IMR) دائمًا أقل من القيم الملاحظة تجريبياً. من بين العديد من النظريات التي تؤخذ في الاعتبار، تقدم NR أفضل تنبؤ لسرعة الصوت. يتناقص تسلسل المؤهلات للتنبؤ بسرعة الصوت نظرًا لأن NR و IMR و FLT غير صالحين تمامًا لجميع الأنظمة المدروسة.

الخلاصة: يزيد التفاعل الجزيئي القوي مع تكوين البنية مع زيادة الكسور الجزيئية. تم العثور على تدمير الأزيوتروبي ليكون الأكثر شيوعًا من المركبات التي تم النظر فيها.

مفاتيح الكلمات: مزيغ ثنائي، تفاعل جزيئي، سرعة الصوت المقدر، نموذج إحصائي.

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