STUDY OF MOLECULAR INTERACTION IN CERTAIN BINARY AND TERNARY LIQUID SYSTEM S BY EXPOSING IT TO ULTRASONIC FREQUENCY OF 2 MHz AT 293.15 K

M.Vijay Alexander[1], S. Sasikumar[2], G. Meenakshi[3]

[1]*Assistant Professor of Physics in V.R.S. College of Engineering & Technology, Arasur, Villupuram*
[2]*Research Scholar in Karpagam University, Coimbatore*
[3]*Associate Professor of Physics (Rtd.) in K.M.C.P.G.S, Government of Pondicherry, Pondicherry*

Abstract

The essential frame work of manufacturing material is composed of scientific and practical interrelationship. It plays the role among the structure, structural properties and performance of all classes of materials that are potentially useful to the society. Even after manufacturing the materials further it is necessary to study the physical and chemical properties of those materials. One of such properties can be studied by exposing the liquid or solid materials to ultrasonic vibrations .In the liquid binary system chosen for this study is toluene with benzene, hexane, heptane and cyclohexane at temperature i.e. 293.15K. The experimental value of ultrasonic velocity and density of binary mixtures are taken from the work of P.S.Nikam etal' and the sample chosen is mainly due to the availability of the experimental data. The various acoustical parameters like ultrasonic velocity, percentage deviation, excess impedance, and excess velocity are calculated and obtained results are suitably interpreted. The ternary system chosen for this study are cyclohexane plus toluene plus 2-propanol, studied at 293.15K.The experimental value of ultrasonic velocity and density for this mixture has been taken from the work of G. Arul etal. The values of sound velocity have been evaluated theoretically using three different methods namely Nomoto, Van-deal and CFT. For both binary and ternary mixtures, the observed result shows that the Nomoto method seems to give good results for the evaluation of acoustical parameters compared to collision factor theory (CFT) and Van-deal's method.

***Key Words**: Binary system, Nomoto method, CFT method, Van-deal's Method.*

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1. INTRODUCTION

The essential frame work of manufacturing material is composed of the scientific and practical interpolation at play among the structure, structural properties and performance of all classes of materials that are potentially useful to the society. Even after manufacturing the materials, it is important that one has to analyze its physical and chemical properties. One such property can be investigated by exposing the liquid and solid materials to ultrasonic sound vibrations. Ultrasonic velocity measurements are widely used to study the physical and chemical behavior of liquid mixtures. In recent years a good amount of work has been done to correlate the experimental ultrasonic velocities with those computed theoretically using empirical and semi empirical relations [1-4]. Nomoto (1958) and Bhimseenachal etal (1962) made successful attempts to evaluate sound velocity on binary liquid mixtures. The free length theory (FLT) of Jacobson (1951, 1952, a, b) and Schaff's (1939) collision factor theory (CFT) have been used to predict intermolecular interactions between unlike molecules of mixtures. Several workers (Pandey etal 1977, 1978, Shukla and Dubey 1984 and Shukla etal (1971) found that FLT is better than CFT for theoretical evaluation of sound velocity whereas Mishra and Pandey (1977) observed that the CFT method is better than FLT for the fore said purpose. Shukla and Dubey (1984) found that the Van-Deal ideal mixing relations given minimum deviation. J.D. Pandey etal[5] found that ideal mixing relation gives the minimum deviation for all the systems except acetone.

These studies motivated the author to find the suitable theoretical method to evaluate the sound velocity in binary and ternary mixture using three different theoretical relations (Nomoto, Van-Deal and CFT)[6].

2. THEORETICAL CONSIDERATIONS

Nomoto [6] suggested an empirical formula for sound velocity in binary liquid mixture as follows;

$$U_m = \left(\frac{X_1 R_1 + X_2 R_2}{X_1 V_1 + X_2 V_2} \right)^3$$

------> (1)

Van-Deal and Van-Deal [7] suggested the following relation for sound velocity U_{im} as

$$\left(\frac{1}{X_1 M_1} \right) \frac{1}{U_m^2} = \left(\frac{X_1}{M_1 V_1^2 + M_2 V_2^2} \right)$$

----> (2)

Jacobson's relation [8] for sound velocity using the concept of intermolecular free length (L_f) is given by,

$$U_{im} = \frac{K}{L_{f(mix)} \rho_{mix}^{1/2}} \quad \text{------> (3)}$$

Where, K is the temperature dependent constant.

Schaff's [9] developed a theoretical formulae for the expansion of sound velocity in binary mixtures as,

$$U_{im} = \frac{U_{\infty}\left(X_1 S_1 + X_2 S_2\right)\left(X_1 B_1 + X_2 B_2\right)}{V_M} \quad \text{------> (4)}$$

The symbols used in all four relations have their usual meaning.

3. Results and Discussion:

The values of sound velocity have been evaluated theoretically using three different methods namely Nomoto, Van-Deal, and CFT. The selected mixture for analysis can be classified as (i) Polar in non polar mixture and (ii) Polar in polar mixture.

3.1 Choice of binary systems:

The binary system chosen for this study is Toluene with Benzene, Hexane, Heptane and Cyclohexane at 293.15K. The experimental value of ultrasonic velocity and density of binary mixture of Toluene with Benzene, Hexane, Heptane and Cyclohexane are taken from the work of P.S. Nikam etal. and the sample chosen is mainly due to the availability of the experimental data. Toluene in Benzene, Hexane, Heptane and Cyclohexane at 293.15K is discussed. The experimental value of density and ultrasonic velocity for pure components of binary and ternary systems are given in the table [1]. The ultrasonic velocity and excess parameters of toluene with other components are given in table 3 and 4. The variation of concentration with ultrasonic velocity of Toluene with different components is reported graphically in figure (1-4).

3.2 Polar in non polar mixture:

Toluene in Benzene, Heptane and Cyclohexane belongs to this category. The calculated values of Umix2/Uidl2 alpha, beta, excess velocity and acoustic impedance for this type of mixtures are given in table [2 & 3]. The variation of excess velocity and beta with the mole fraction of Toluene is given in fig (5). From the table (2), it is observed that the average percentage deviation of computed ultrasonic velocity using various theories like Nomoto method, Van-deal's ideal mixing method and collision factor theory for the mixtures of Toluene with Benzene are 0.20, 0.20 and 0.55 at the temperature 293.15K. For the binary mixture Toluene with Heptane the average percentage deviations are 0.65, 1.70, and 5.39 at the temperature 293.15K,whereas for the binary mixture Toluene with cyclohexane the average percentage deviations are 1.07, 0.90 and 4.1 at 293.15K .The percentage deviation can be studied on the basis of interaction between the components of mixture. Normally in polar and non-polar mixture there is dipole-induced dipole interaction which is very weak10&11. Toluene is associated through hydrogen bonding. The mixing of toluene with non polar may results in the breaking of hydrogen bond, thereby promoting dissociation. The positive deviation observed is due to the molecular association and complex formation of molecules where as the negative deviations are due to the molecular dissociation of associative molecules. The magnitude of deviation also depends on concentration12&13.In the case of Toluene in Benzene and in Heptane it is found to be less in Nomoto method compared to Van- Deal and CFT method. At higher temperature the deviations do not show smooth variation. So, Nomoto method gives best result in these mixtures. In the case of Toluene in cyclohexane the deviations are found to be less in Nomoto method compared to Van- Deal and CFT method. Since, the adiabatic compressibility decreases gradually in its value with the increase of mole fraction, Van-Deal method gives best result in this mixture.

3.3 Polar in Polar mixture:

Toluene in Hexane belongs to this category. The calculated of U2exp/U2idl , α, β, excess velocity and acoustic impedance for this type of mixture are given in table (3) for Toluene in Hexane at 293K. The variation of excess velocity with the mole fraction of toluene in Hexane is shown in the figure (6). From the tables it is observed that the average percentage deviation of computed ultrasonic velocity using various theories namely Nomoto method, Van-Deal ideal mixing method and CFT method for the mixture of Toluene with Hexane are 0.61, 0.47, and 1.75 at the temperature 293.15K. Toluene in Hexane is found to have a weak dipole-dipole interaction. At low temperature, a very few deviations are found to be negative in both Nomoto and Van- Deal methods. But CFT method shows positive deviations only. Analyzing the percentage deviation of Toluene in Hexane, Van-Deal gives best result at low temperatures and Nomoto method gives good result at high temperature.

3.4 Choice of ternary systems:

The ternary systems chosen for this study are Cyclohexane + Toluene + 2-propanol at 293.15K.The experimental value of ultrasonic velocity and density of this ternary mixture are taken from the work of G.Arul etal. . The experimental value of density and ultrasonic velocity for pure components are given in the table (1). From the experimental values in the above mixture of different mole fraction of Cyclohexane and 2-propanol at 293.15K has been reported in table (1). The variation of ultrasonic velocity, β and excess velocity with concentration of cyclohexane and 2-propanol is reported graphically in figures (7,8). Cyclohexane is a non polar liquid where as toluene and 2-propanol is polar liquids. The calculated values of alpha, beta, excess velocity and excess impedance are positive and decreases in concentration of 2-proponol. Since the components are

having Zero dipole moments, the dipole-dipole interaction14 is weak in pure state. The decrease in magnitude of the excess parameters suggests the close packing of molecules inside the shield, which may be brought about by the increasing magnitude of interaction15&16. The positive and decrease of excess parameters with increase of 2-propanol concentration is due to a weak bond between a conventional localized hydrogen bond and the formation of charge transfer complex occurring between the components of the mixtures17&18. The excess volume studies also confirm the weakening of the dipolar interaction between the components of the liquid mixture19. The increase of concentration in ternary mixtures reduces the beta value which shows that there is a strong interaction in the liquid mixtures.

Table (1): Ultrasonic velocity and Density of pure components for Binary and Ternary mixtures: (293.15K)

	293.15K	
Component	Density $\rho 10^3$ kg m^{-3}	Velocity Ums^{-1}
Toluene	867	1312.4
Benzene	879	1308.5
Heptane	682	1150.2
Cyclohexane	779	1274.6
Hexane	658	1098.0
2-propanol	768.5	1141.3

Values taken from the work of P.S. Nikam etal and G.Arul etal.

Table (2): Excess parameters in the ternary mixture: (293.15K)

Mole fraction X_1	Mole fraction X_2	Ultrasonic velocity U_{idl} ms^{-1}	Uexpt^2/ $U_{idl}{}^2$	α	β x 10^{-10}	Excess velocity (u^E) ms^{-2}	Excess impedance Z^E 10^3kg/m2/ s
0.400	0.199	1249.9	0.980	-0.0196	7.832	-12.3	10.88
0.200	0.400	1205.4	1.0414	0.0414	8.355	24.7	9.928
0.100	0.499	1186.0	1.0696	0.0696	8.593	40.6	9.811
0.001	0.599	1173.2	1.0874	0.0874	8.747	50.2	9.744

Table (3): Ultrasonic velocity of Binary mixtures: (293.15K)

Binary mixtures	Mole fraction X_1	U_{exp*} ms^{-1}	Nomoto ms^{-1}	Van-Deal ms^{-1}	CFT ms^{-1}	Percentage Deviation		
						$\Delta U/U_{exp}$% Nomoto	$\Delta U/U_{exp}$% Van-Deal	$\Delta U/U_{exp}$% CFT
	0.0412	1270.4	1273.7	1271.6	1261.3	0.25	0.09	0.71
	0.1729	1274.4	1273.1	1274.5	1268.1	0.10	0.07	0.49
Toluene	0.3580	1277.3	1276.1	1276.6	1270.7	0.08	0.53	0.51
+ benzene	0.5565	1280.7	1278.1	1273.5	1277.1	0.20	0.58	0.28
	0.6623	1305.0	1289.1	1277.6	1287.1	1.21	2.09	1.37
	0.0677	1161.2	1158.1	1147.6	1101.2	0.23	1.17	5.16
	0.2560	1192.0	1195.6	1183.4	1134.2	0.30	1.31	5.40
Toluene	0.4798	1238.6	1233.6	1216.0	1172.0	0.40	1.82	5.37
+ Heptane	0.6744	1281.6	1266.0	1254.7	1206.1	1.21	2.09	5.89
	0.8465	1322.1	1308.4	1296.6	1251.5	1.02	1.93	2.33
	0.0677	1125.7	1118.6	1120.3	1110.2	0.63	0.47	1.37
Toluene +	0.2566	1158.3	1146.2	1150.1	1140.3	1.04	0.70	1.55

Cyclohexane	0.4793	1195.8	1175.2	1189.3	1186.4	1.70	0.54	0.77
	0.6744	1228.5	1215.4	1210.5	1220.7	1.06	1.46	0.63
	0.8467	1258.3	1241.9	1240.6	1240.6	1.30	1.40	1.12
	0.0609	1070.9	1075.6	1069.0	1055.4	-0.43	0.17	1.44
Toluene	0.2355	1106.1	1101.1	1083.1	1096.2	0.42	0.07	0.89
+ Hexane	0.4509	1161.1	1150.0	1129.8	1130.4	0.96	0.47	2.64
	0.6489	1199.6	1184.0	1169.8	1180.0	1.30	1.10	1.63
	0.8313	1238.0	1226.1	1230.2	1211.4	0.96	0.61	2.15

Table (4): Excess parameters in the Binary mixture: (293.15K)

Mixture	Mole fraction X_1	Ultrasonic velocity U_{idl} ms^{-1}	U^2_{exp}/U^2_{idl}	α	β x 10^{-10}	Excess velocity (u^E) ms^{-2}	Excess impedance Z^E 10^3kg/m2/ s
Toluene + Benzene	0.0412	1271.6	0.9980	-0.0020	7.2007	-1.25	10.92
	0.1729	1274.5	0.9998	-0.0002	7.1823	-0.09	10.92
	0.3580	1274.6	1.0010	0.0012	7.1778	0.68	10.91
	0.5565	1273.2	1.0118	0.0118	7.2352	7.50	10.85
	0.7699	1277.6	1.0433	0.0433	7.2045	27.39	10.86
Toluene + Heptane	0.0677	1147.6	1.0238	0.0238	10.856	13.6	8.026
	0.2560	1183.4	1.0268	0.0268	09.826	15.8	8.599
	0.4798	1216.0	1.0375	0.0375	08.875	41.1	9.608
	0.6744	1254.7	1.0433	0.0433	07.994	26.9	9.969
	0.8461	1296.6	1.0397	0.0397	07.157	25.5	10.77
Toluene + Cyclohexane	0.0677	1120.3	1.0096	0.0096	11.772	5.4	7.582
	0.2566	1150.1	1.0013	0.0143	10.741	8.2	8.094
	0.4793	1189.3	1.0019	0.0109	09.555	6.5	8.797
	0.6744	1210.5	1.0299	0.0299	08.795	7.8	9.392
	0.8467	1240.6	1.0287	0.0287	08.001	17.7	9.840
Toluene + Hexane	0.0609	1069.0	1.0035	0.0035	13.380	1.89	6.990
	0.2355	1105.2	1.0015	0.0115	11.856	0.87	7.566
	0.4509	1155.6	1.0096	0.0096	10.320	5.55	8.384
	0.6489	1186.3	1.0225	0.0225	09.272	13.3	9.091
	0.8313	1230.6	1.0124	0.0124	08.182	7.62	9.932

Fig (1)

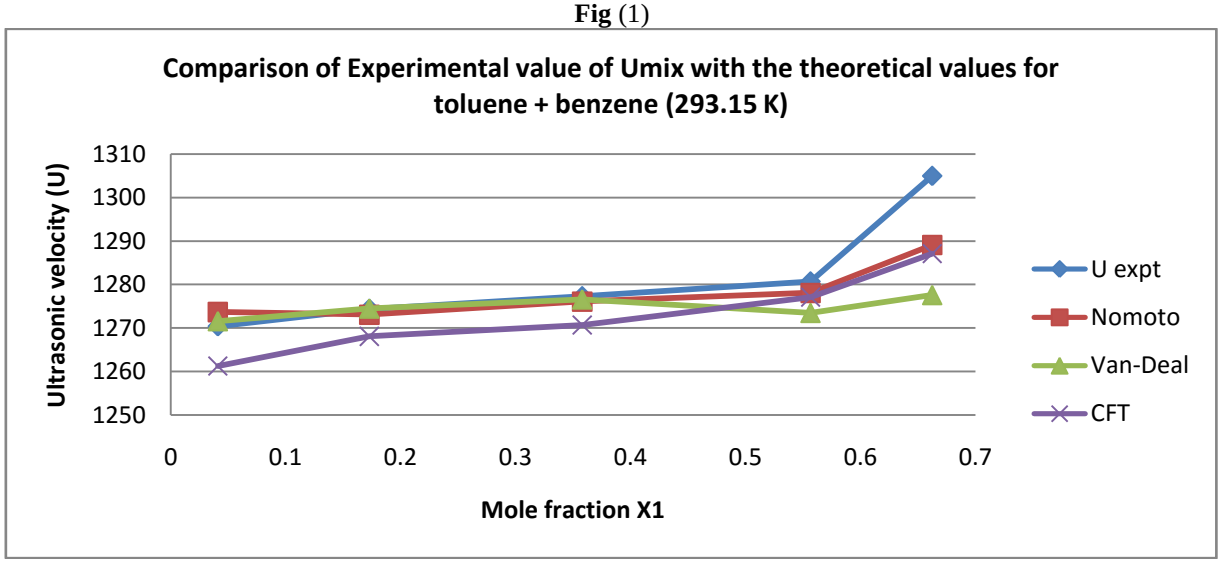
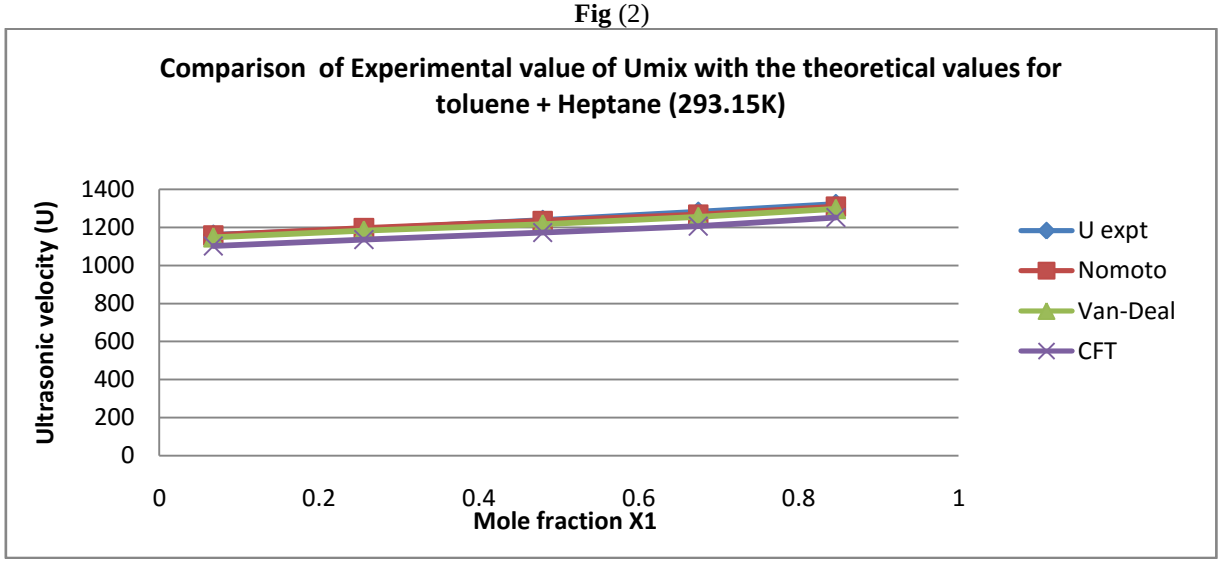


Fig (2)



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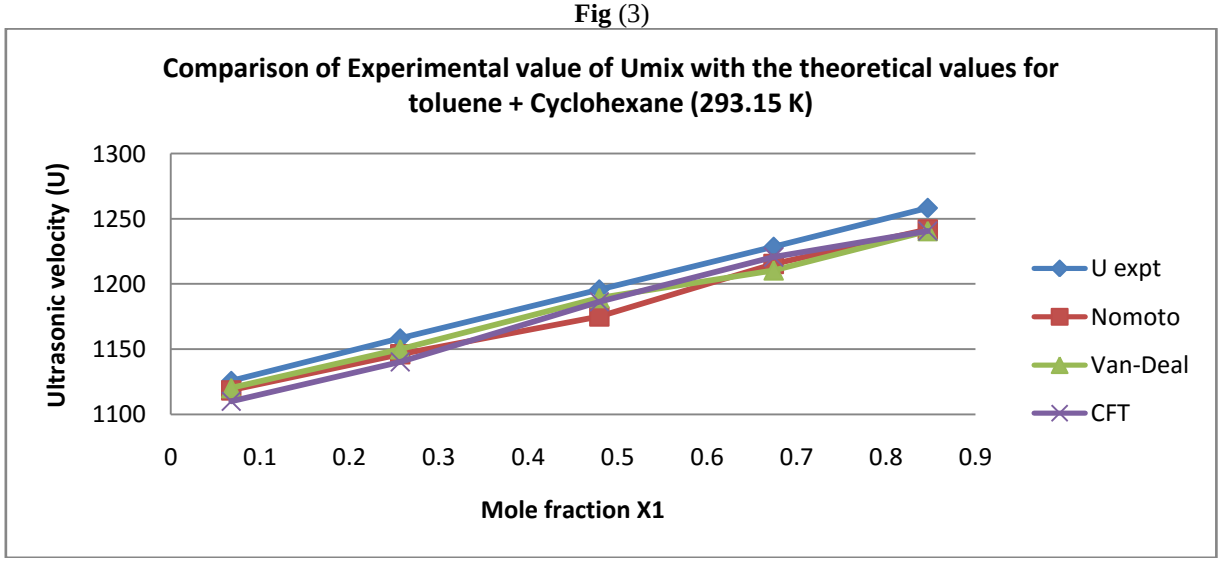

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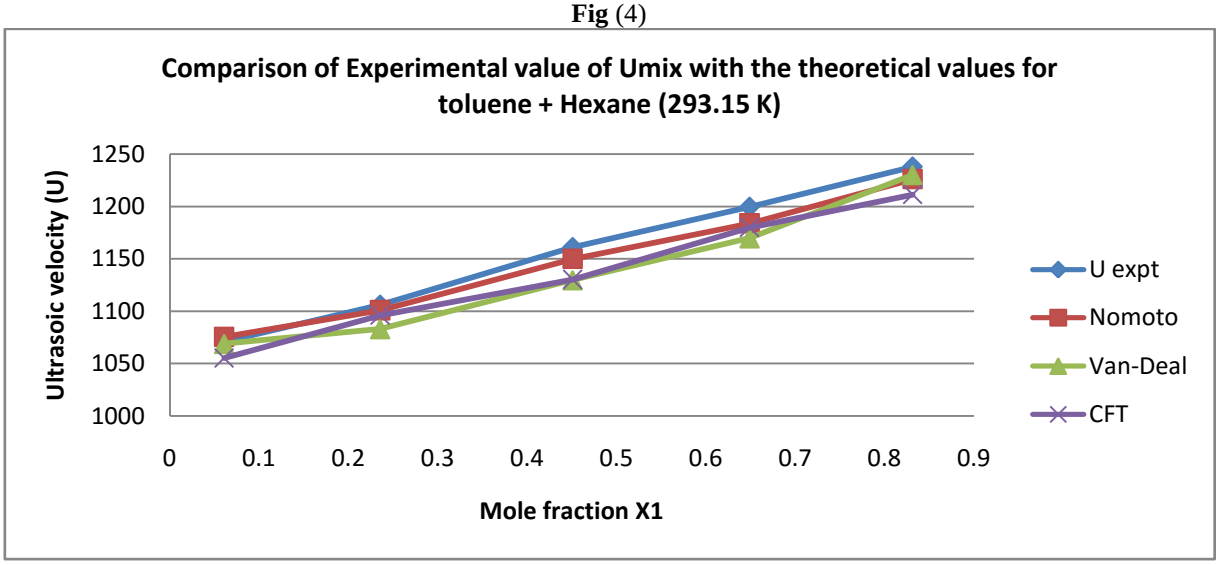

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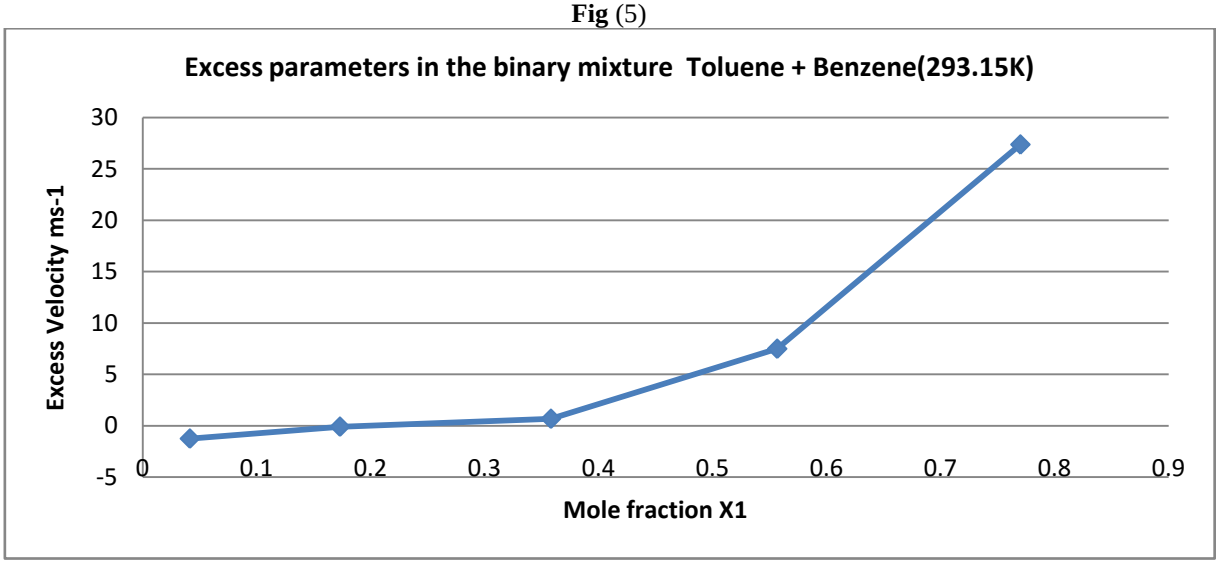

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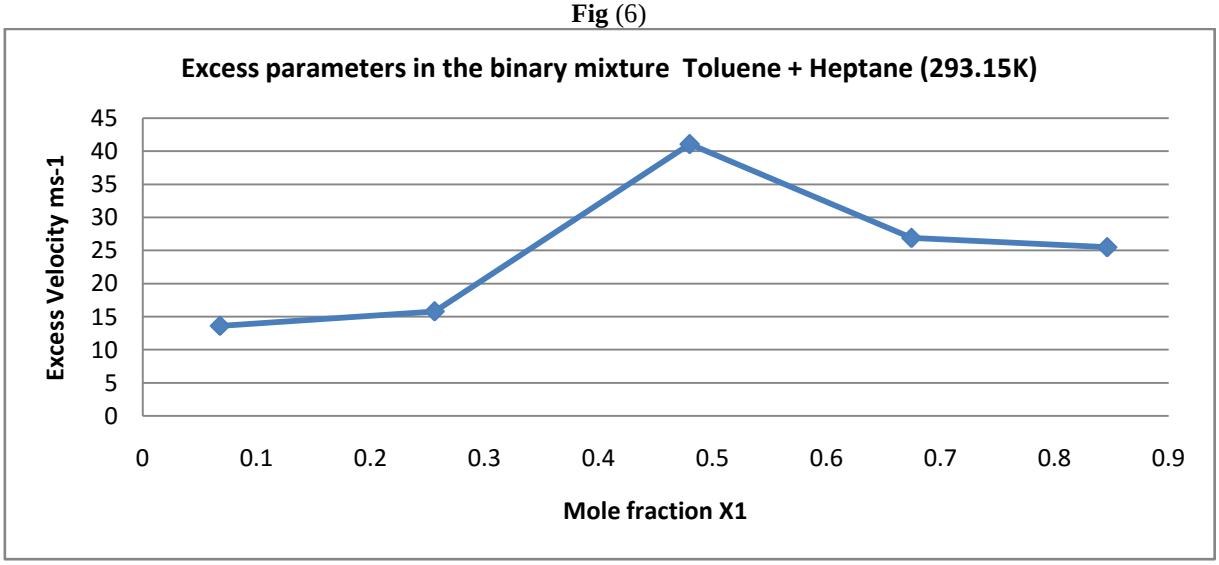

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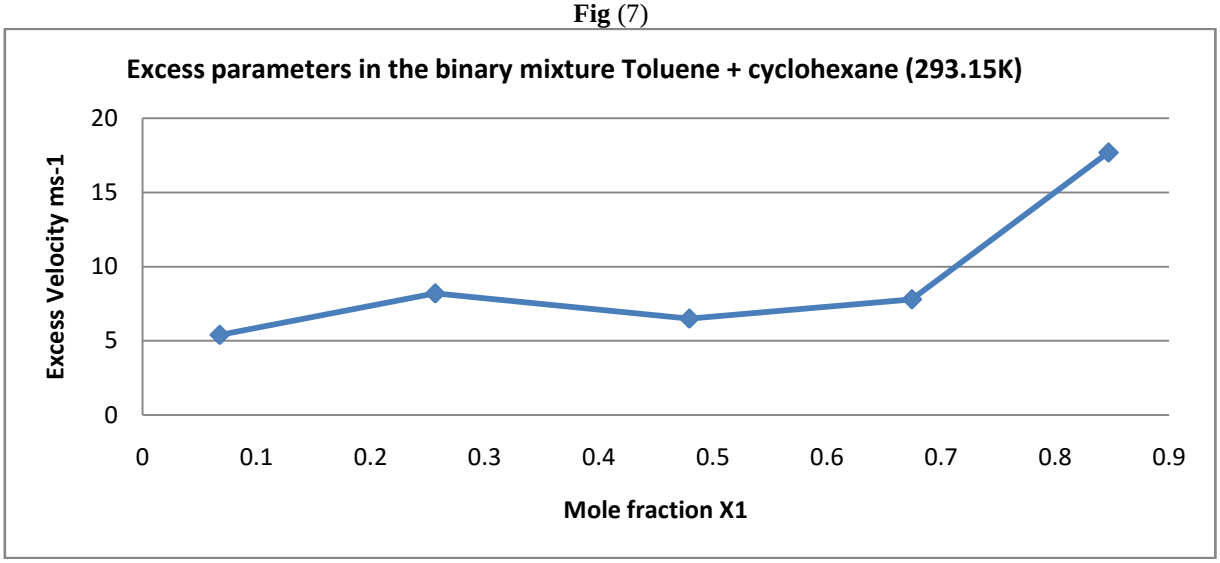

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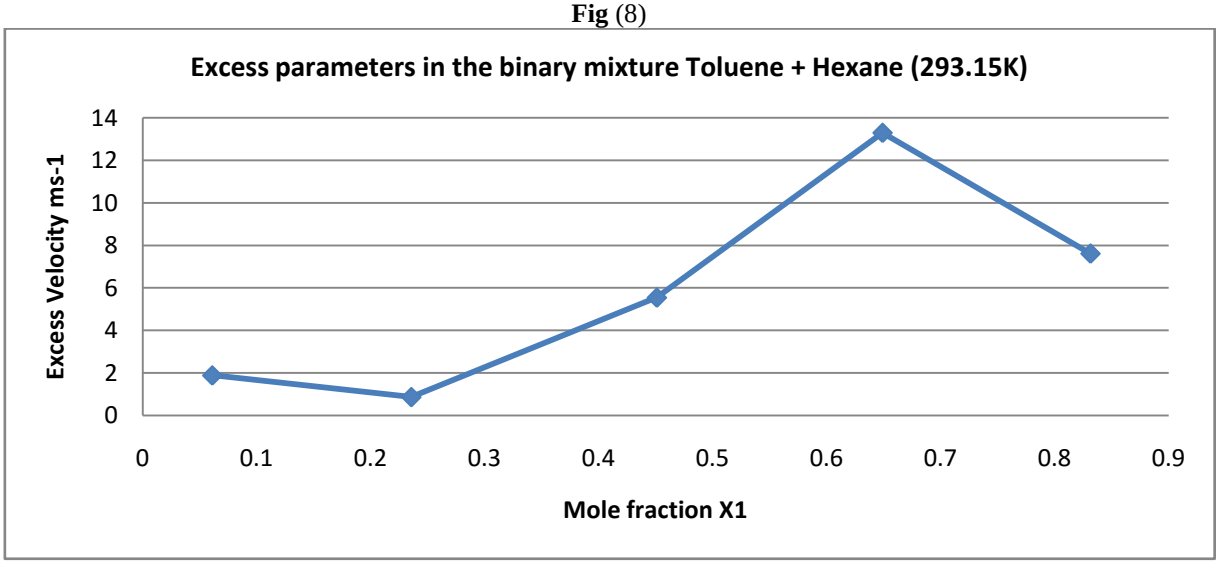

CONCLUSION

The percentage deviation can be studied on the basis of interaction between the components of mixtures. Normally in polar and non polar mixtures there is dipole-induced dipole which is very weak. This type of mixture also results in the breaking of hydrogen bond thereby promoting dissociation. The positive deviation observed is due to the molecular association and complex formation of molecules, whereas the negative deviation is due to the molecular dissociation of associative molecules. The magnitude of deviation also depends on concentration. In ternary mixture the decrease of magnitude of excess parameter suggest the close packing of molecules inside the shield which may be brought about by the increase in magnitude of interaction. The increase of concentration in ternary mixture reduces the beta value which shows that there is strong interaction in liquid mixtures. This work is found to be quite interesting and out of three different methods Nomato methods is found to be the best one due to the closeness of the value observed with respect to the experimental one.

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