Theoretical evaluation of Ultrasonic velocity in Binary mixtures of an edible oil with alkyl Acetates

Suhashini Ernest[1] and P. Kavitha[2]

[1]P. G and Research Department of Physics, Urumu Dhanalakshmi College, Tiruchirappalli, Tamil Nadu. India.
[2] Department of Physics, Indra Ganesan College of Engineering, Tiruchirappalli, Tamil Nadu India.
*E-mail: pkavithaa@yahoo.com

ABSTRACT

The ultrasonic velocity in binary liquid mixtures of an commonly used edible oil with organic solvents, butyl acetate and ethyl acetate are measured over the entire range of concentrations at 298.15 K. The theoretical values of ultrasonic velocity for the binary mixture for the same mole fractions have been evaluated using various theoretical models and empirical relations like Nomoto's relation, Danusso model and Junjie's Relation. The estimated theoretical values are compared with the calculated experimental values and the Chi-square test for goodness of fit is applied and the validity of these theories and relations are discussed.

Keywords: ultrasonic velocity, sesame oil, butyl acetate, ethyl acetate, chi-square test.

INTRODUCTION

The binary mixtures rather than pure components are of great practical importance in most chemical, industrial and biological processes, as they provide large applications with the desired properties. The oil industry is always in demand of physico-chemical and thermo dynamical properties of various oils and their mixtures with different organic solvents. The ultrasound velocity measurements are helpful to study the intermolecular interactions and thermo dynamical properties of pure components and their mixtures[1]. Sesame oil has been used as edible oil for thousands of years. The lignans present in sesame oil are thought to be responsible for many of its unique chemical and physiological properties, including its antioxidant and antihypertensive properties[2,3]. It is found that less work have been made on the thermodynamics of mixture of oil with organic solvents. In the present study an attempt has been made to study the intermolecular interactions in the binary mixtures of sesame seed oil with acetates by measuring the ultrasonic velocity and density of the mixtures at 298.15K. Various theories and relations suggested by Nomoto[4], Danusso[5] and Junjie[6] are used to calculate the ultrasonic velocity.

MATERIALS AND METHODS

Chemicals used in the present research work are AR grades obtained from Merck. The purities of the above chemicals were checked by density determination at 298.15 K and compared with the literature values (Table 1). The weight of the sample was measured using electronic digital balance with an accuracy of ± 0.1 mg (Shimadzu AX-200). An ultrasonic interferometer having with frequency of 2 MHz (Mittal) with an accuracy of ± 0.1 m/s has been used for measurement of velocity. An electronically operated constant temperature bath (RAAGA) has been used to with an accuracy of ± 0.01 K to maintain constant temperature

Sesame seed oil was supplied by Bunge (Tamil Nadu) and from the fatty acid composition the average molar mass of the sesame seed oil has been computed as 875.40 g/mol.

Table-1: Physical properties of liquids used in this work at 298.15K

Components	ρ (gm/cm^3)		u (m/s)	
	Experimental	Literature[7]	Experimental	Literature[9]
Sesame Oil	0.91579	0.915-0.925[8]	1456.0	-
Butyl acetate	0.87661	0.87636	1192.0	1190.0
Ethyl acetate	0.89507	0.89455	1147.5	1148

Theory and Calculations

The ultrasonic velocity in binary mixtures can be evaluated theoretically using the following theories and empirical relations.

Velocity due to Nomoto is given by the empirical relation,

$$U_{NR} = \left(\frac{x_1 R_1 + x_2 R_2}{x_1 V_1 + x_2 V_2}\right)^3 \qquad \ldots\ldots\ldots\ldots\ldots (2)$$

where x_1 and x_2 are the mole fractions of pure components in the binary mixtures, R and V represents the molar sound velocity and molar volume.

Velocity of ultrasonic waves according to Danusso model is given by the formula

$$U_{DM} = \frac{1}{\rho_{mix}} \left(\frac{1}{M_{eff}} \left(\frac{x_1 M_1}{\rho_1^2 u_1^2} + \frac{x_2 M_2}{\rho_2^2 u_2^2}\right)\right)^{-1/2} \qquad \ldots\ldots\ldots\ldots\ldots (3)$$

where M_{eff} is the effective molecular weight and others have usual meaning.

Velocity according to Junjie's relation is given by the expression,

$$U_{JR} = \frac{x_1 V_1 + x_2 V_2}{(x_1 M_1 + x_2 M_2)^{1/2}} \left(\frac{x_1 V_1}{\rho_1 u_1^2} + \frac{x_2 V_2}{\rho_2 u_2^2}\right)^{-1/2} \qquad \ldots\ldots\ldots\ldots\ldots (4)$$

Chi-square value is calculated using the formula,

$$\chi^2 = \sum_{i=1}^{n} \frac{\left(U_{exp} - U_{cal}\right)^2}{U_{cal}} \qquad \ldots\ldots\ldots\ldots\ldots (5)$$

Where n is the number of data points.

The Average Percentage Error is given by the formula,

$$APE = \frac{1}{n} \sum \frac{U_{exp} - U_{cal}}{U_{exp}} \times 100\% \qquad \ldots\ldots\ldots\ldots\ldots (6)$$

Where U_{exp} are the experimental values of velocities and U_{cal} are theoretical values of velocities.

RESULTS AND DISCUSSION

The ultrasonic velocity and density for the binary mixture of sesame seed oil with butyl acetate and ethyl acetate are measured experimentally. The experimental and theoretically calculated values using different models of mixtures prepared using the solvents butyl acetate and ethyl acetate are presented in tables 2 and 3. The validity of the theoretical values is verified by using Chi-square test by calculating Average Percentage Error.

Table-2: Values of experimental and theoretical Ultrasonic velocity of the (Butyl acetate(x_1) + sesame oil) at 298.15K.

Mole Fraction	Ultrasonic Velocity (m/s)				Modulus of Percentage Deviation		
X1	U_{Exp}	U_{NR}	U_{DM}	U_{JR}	U_{NR}	U_{DM}	U_{JR}
0.0991	1451.2	1451.77	1450.02	1450.40	0.04	0.08	0.06
0.2068	1444.0	1446.19	1442.33	1443.09	0.15	0.12	0.06
0.3017	1436.0	1440.13	1434.44	1435.28	0.29	0.11	0.05
0.4022	1428.0	1432.09	1424.36	1425.10	0.29	0.25	0.20
0.4990	1412.6	1422.08	1411.88	1412.70	0.67	0.05	0.01
0.5996	1400.0	1408.09	1394.90	1395.89	0.58	0.36	0.29
0.6999	1379.2	1388.23	1371.86	1372.96	0.66	0.53	0.45
0.8028	1352.0	1356.69	1337.27	1338.65	0.35	1.09	0.99
0.9005	1304.0	1304.76	1285.91	1287.10	0.06	1.39	1.30
0.9792	1231.0	1225.07	1217.05	1217.83	0.48	1.13	1.07

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Table-3: Values of experimental and theoretical Ultrasonic velocity of (Ethyl acetate(x_1) + sesame oil) at 298.15K.

Mole Fraction	Ultrasonic Velocity (m/s)				Modulus of Percentage Deviation		
X_1	U_{Exp}	U_{NR}	U_{DM}	U_{JR}	U_{NR}	U_{DM}	U_{JR}
0.0994	1450.1	1452.26	1450.83	1450.92	0.15	0.05	0.06
0.1958	1448.0	1447.86	1444.97	1445.01	0.01	0.21	0.21
0.2986	1440.0	1442.05	1437.15	1437.29	0.14	0.20	0.19
0.3986	1428.8	1434.81	1427.64	1427.83	0.42	0.08	0.07
0.4984	1416.0	1425.28	1415.48	1415.63	0.66	0.04	0.03
0.5996	1400.0	1411.92	1398.68	1398.97	0.85	0.09	0.07
0.6990	1376.0	1392.62	1375.47	1375.79	1.21	0.04	0.02
0.7996	1344.0	1361.08	1339.68	1339.98	1.27	0.32	0.30
0.8999	1276.0	1301.59	1278.23	1278.53	2.01	0.17	0.20
0.9798	1181.7	1195.59	1184.68	1184.77	1.18	0.25	0.26

Table-4: Values of Chi-Square test and Average Percentage Error of ultrasonic velocity for binary mixtures at 298.15K

Theories	Butyl acetate + sesame oil		Ethyl acetate + sesame oil	
	χ^2	APE	χ^2	APE
Nomoto	0.0241	0.36	0.1269	0.79
Danusso	0.0649	0.51	0.0040	0.14
Junjie	0.0545	0.45	0.0038	0.14

It is evident from the examination of the tables 2 and 3 that when the concentration of the solvent in the mixtures increases the speed of sound is found to decrease. It is observed that the experimental values show deviation (Figure 1 and 2) with the theoretical values of ultrasonic velocities which confirms the existence of molecular interactions. The reason may be the limitations and approximations incorporated in these theories.

From the table 4, it is seen from the results for the butyl acetate + sesame oil mixture, the theories are in the order of NR, JR, and DM and for ethyl acetate + sesame oil mixture it is in the order of JR, DM, and NR.
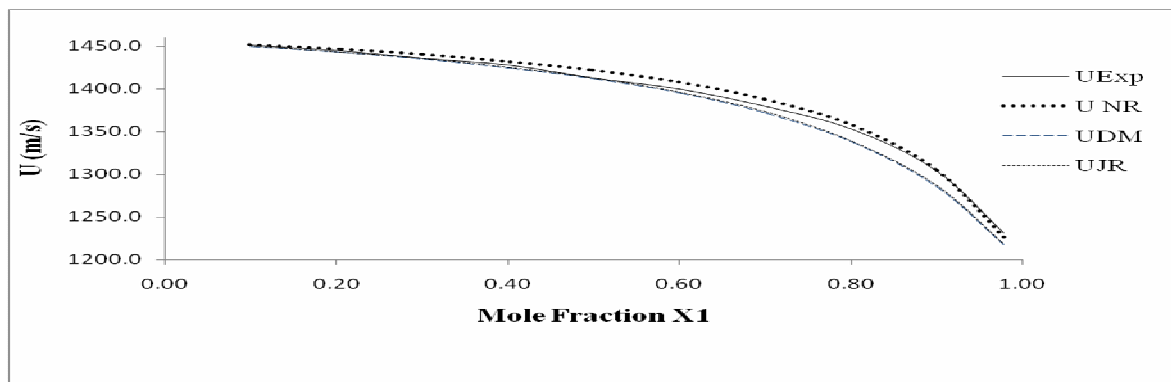

Fig.-1: Variation of Experimental values of ultrasonic velocity with theoretical values (NR,DM,JR) for binary mixture of Butyl acetate(X1)+Sesame oil (X2)
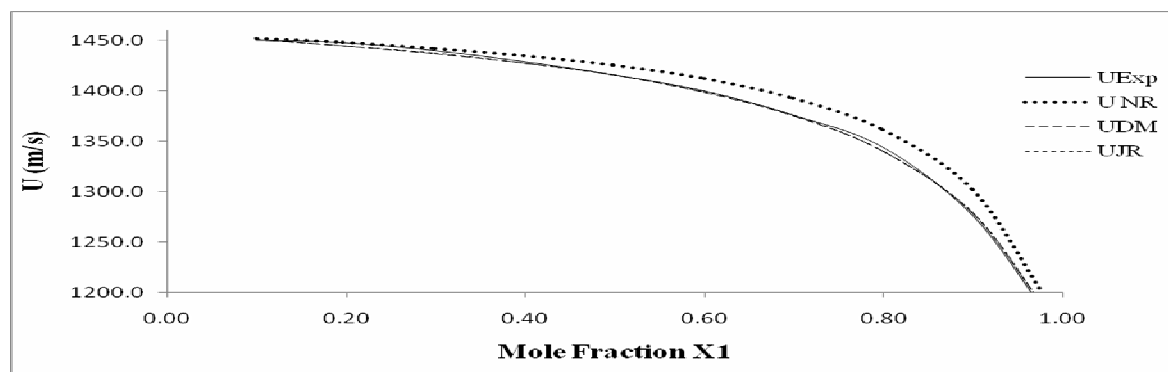
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Fig.-2: Variation of Experimental values of ultrasonic velocity with theoretical values (NR, DM and JR) for binary mixture of Ethyl acetate(X1) +Sesame oil (X2)

CONCLUSION

The measurement of ultrasonic velocities for binary mixtures of acetates with sesame oil was compared with the various theoretical models like Nomoto, Danusso and Junjie at 298.15K. From the observation it is found that Nomoto is best suited with the experimental values for butyl acetate mixture and junjie's model are best suited for ethyl acetate mixture.

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