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Viscometric and speed of sound studies of the binary liquid mixtures of acetone with 2-propanol at 303.15K

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Abstract: *The speed of sound (U), density (ρ) and viscosity (η) has been measured for the mixtures of acetone with 2-propanol at T = 303.15 K. The experimentally determined values of speed of sound have been used to check the applicability of different speed of sound models of nomoto (NOM), impedance (IMP), vandael and vangeel (VDV), junjie (JUN) and rao's specific velocity (RAO) relation. The validity of the theories was checked by applying the chi-square test (χ) for goodness of fit and by calculating the average percentage error (APE).Further Viscosity data have been used to test the applicability of standard viscosity models of Hind,Grunberg and Nissan, Katti and Chaudhri, Tamura &Kurata, after that corresponding interaction terms and standard deviation (σ) of these theories are calculated at various temperatures for the binary liquid systems . The results are interpreted in terms of molecular interaction between the components of the mixtures.*

Keywords: *speed of sound, chi-square test, average percentage error, viscosity and standard deviation.*

I. Introduction

Thermodynamic properties are important has been given to the behavior of mixed components rather than the single component because of their widespread range of applications. The practical need for thermodynamic data for investigation and research as well as for design and set up of industrial processes continue to drive research in the study of multi component systems. Thermodynamic properties derived from the measurement of ultrasonic velocities, densities and viscosities for binary mixtures are useful in understanding the nature and type of intermolecular interactions present between the constituent molecules.

In the present investigation, experimentally determined ultrasonic sound velocities are compared with the theoretical relations like nomoto (NOM), impedance (IMP), vandael and vangeel (VDV), junjie (JUN) and rao's specific velocity (RAO) relation at 303.15K temperature.The deviation in the variation of average percentage error, (APE), Chi-square test for goodness of fit, from unity have also been evaluated ("equations 1-7")to explain the non-ideality of the system.

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Further, the mixture viscosities were correlated using Hind,Grunberg and Nissan, Katti and Chawdhry ,Tamura &Kurata, equations to test their relative applicability with standard deviation(σ) ("equations 8-12") for the binary mixture of acetone with 2-propanol at different mole fractions, the results are explained and discussed in terms of molecular interactions present in the investigated systems.

II. Experimental

The ultrasonic velocity was measured at 303.15K using ultrasonic interferometer (M/s Mittal Enterprises, India) operating at a frequency of 2 MHz with an accuracy of ±0.1m/s. for the compounds of acetone with 2-propanol .

The density was measured by using specific gravity bottle method and Viscosity was measured by using Ostwald's viscometer by the standard procedure.

Table 01 Comparison of experimental densities ( ), viscosities ( ) and speed of sound (U) of pure liquids with literature values

liquid	Temp T (K)	Density(ρ) kg m^{-3}		Viscosity(η) $kgm^{1}s^{-1}$		Speed of sound(U) $m.s^{-1}$	
		literature	**experimental**	**literature**	**experimental**	**literature**	**Experimental**
Acetone	303.15	0.7860[a]	0.7865	3.73[b]	3.77	1138.00[c]	1138.20
2-propanol	303.15	0.7810[d]	0.7817	1.52[e]	1.52	1107.80[f]	1107.80

[a,b,c] Reference [3]
[d,e,f] Reference [1]

III. Theory

Several semi empirical relations have been proposed by many researchers for the computation of ultrasonic velocity and viscosity for binary component system. In the present paper the following equations are used, they are

Ultrasonic theories;

3.1 Nomoto's relation : Nomoto derived a relation to evaluate ultrasonic velocity for a multi component liquid solutions and which can be expressed as,

$$U_{NOM}=[X_1R_1+X_2R_2/X_1V_1+X_2V_2]^3 \quad (1)$$

Where R = V.U where $V = M_{eff}/\eta$

Where X, R and V are the mole fraction, molar sound velocity and molar volume of the mixture

3.2 Junjie's method : The Junjie's relation for the determination of ultrasonic velocity for the multicomponent mixtures can be expressed as,

$$U_{JM}=[X_1V_1+X_2V_2/(X_1m_1+X_2m_2)^{1/2}][X_1V_1/d_1U_1^2+X_2V_2/d_2U_2^2]^{-1/2} \quad (2)$$

Where X, d, U and V are the mole fraction, density, ultrasonic velocity and molar volume of the mixture

3.3 Imedance relation: The sound speed in the mixture is given by Impedance dependence relation can be expressed as

$$U_{IMP}=X_1Z_1+X_2Z_2/X_1\rho_1+X_2\rho_2 \quad (3)$$

WhereX, ρ and Z are the mole fraction, density and acoustic impedance of the mixture.

3.4 Vandael & Vangeel relation: The Van Dael and Vangeel in the light of assumptions made by Blandermer and Waddington, yield the following relation for ultrasonic velocity in liquid mixtures expressed as

$$U_{VDV}=[1/X_1m_1+X_2m_2]1/2[X_1/m_1U_1^2+X_2/m_2U_2^2]^{-1/2} \quad (4)$$

Where X, m and U are the mole fraction, effective molecular weight and ultrasonic velocity of the mixture

3.5 Rao's relation : Rao's relation is also called as specific sound velocity and can be expressed as

$$U_R = (R/V)^3 \quad (5)$$

Where R ,V are the Rao's specific sound velocity and molar volume of the mixture

3.6 The validity of the theories is checked by applying Chi-square test and by calculating average percentage error, the relations as follows

APE $= [(1/(n)\sum 100(Uexp$ - Ucal)/Uexp)] x 100% (6)

Chisquare(χ) $= \sum_{i=1}^{n}(Uexp$- Ucal)^2/Ucal)] (7)

Where, *n*- number of data used

Viscosity theories;

3.7 Hind equation: Hind's proposed the following equation

$$\eta = x_1^2\eta_1 + x^2{}_2\eta_2 + 2x_1x_2H_{12} \quad (8)$$

Where H_{12} is attributed to unlike pair interactions

3.8 Katti &Chawdhry equation : Katti &Chawdhry derived the following equation

$$\ln\eta V = x_1 \ln \eta_1V_1 + x_2 \ln \eta_2V_2 + x_1x_2W\text{vis}/RT \quad (9)$$

where Wvis is an interaction term and υ is the molar volume of pure component

3.9 Gruenberg-Nissan equation : Gruenberg-Nissan provided the following equation

$$\ln \eta_{12} = x_1 \ln \eta_1 + x_2 \ln \eta_2 + x_1x_2G_{12} \quad (10)$$

where G_{12} is an approximate measure of the strength of the interaction between the components

3.10 Tamura and Kurata equation: Tamura and Kurata gave the following equation

$$\eta_m = x_1\eta_1\Phi_1 + x_2\eta_2\Phi_2 + 2(x_1x_2\Phi_1\Phi_2)^{1/2}T_{12} \quad (11)$$

where Φ_1 and $\Phi2$ are the volume fractions of components 1 and 2, respectively; T_{12} is Tamura

and Kurata constant

3.11 The standard deviation: The correlating ability of each equations from (8) – (11) was tested by a standard deviation (σ)equation

$$\sigma = [(1/(n-k)\ \sum 100(\eta exp\ - \eta cal)/\eta exp)^2\ ]^{1/2} \qquad (12)$$

where n represents the number of data points and k is the number of numerical coefficients .

IV. Results & Discussions

The study of thermo-acoustical and excess thermo-acoustical parameters are useful to explain strength of the interactions between the component molecules of liquid mixtures in most of the cases. But in some cases where there is no possibility for the calculation of acoustical and theoretical speed of sound and viscosity studies play the major role. Hence this kind of evaluation of theoretical speed of sound values proves to be useful to verify the applicability of various postulates of these theories of liquid mixtures and to arrive at some useful inferences regarding the strength of molecular interactions between component liquids in some cases.

The empirical relations due to Nomoto's relation, Impedance relation, Junjie's method vandael and vangeel theory and Rao's are employed and the Average percentage error along with the Chi square fit values of these theories for these liquid mixtures are compiled in Table- 02 .The average percentage error values are small and negative. On comparison, the Nomoto's relation and impedance relation are found to give some valuable estimate of the experimental values of speed of sound values in these mixtures. The predictive abilities of various speeds of sound theories depend upon the strength of interaction prevailing in a system. The extent of deviation may be attributed to the assumptions made in these theories for the non polar- polar and non polar-non polar interaction between the molecules. The Chi-square value is minimum for Nomoto's relation and Junjie's method than those obtained by other theories. An important reason for deviation from experimental values of speed of sound is that the molecular association effects are not taken into account in these theories.

Table 02 Speed of sound theories of acetone with 2-propanol at 303.15 K temperature

X_1	U_{EXP} m.s^{-1}	U_{NOM} m.s^{-1}	U_{IMP} m.s^{-1}	U_{JM} m.s^{-1}	U_{VDV} m.s^{-1}	U_R m.s^{-1}
0.0000	1107.8	1107.8	1107.8	1107.8	1107.8	1107.8
0.1025	1088.6	1110.8	1110.9	1110.7	1110.8	1110.9
0.2045	1091.4	1113.8	1114.0	1113.6	1113.8	1116.5
0.3059	1098.2	1116.8	1117.1	1116.5	1116.9	1119.7
0.4067	1107.8	1119.8	1120.2	1119.5	1119.9	1123.2
0.507	1111.2	1122.8	1123.3	1122.5	1123.0	1125.9
0.6067	1115.6	1125.9	1126.3	1125.6	1126.0	1128.6
0.7058	1122.2	1128.9	1129.3	1128.7	1129.0	1130.9
0.8044	1126.4	1132.0	1132.3	1131.8	1132.1	1133.2
0.9025	1130.8	1135.1	1135.3	1135.0	1135.1	1135.9
1.0000	1138.2	1138.2	1138.2	1138.2	1138.2	1138.2
APE		-0.0026	-0.0027	-0.0026	-0.0027	-0.0033
CHI TEST(χ)		0.1205	0.1295	0.1147	0.1240	0.1920

Several semi empirical relations have been used to represent the dependence of viscosity on concentration of components in binary liquid mixtures, and these are classified according to the number of adjustable parameters used to account for the deviation .We will consider here some of the most commonly used semi empirical models for analyzing viscosity of liquid mixtures based on one, two, and three parameters has been made to check the suitability of equations for experimental data fits by taking into account the number of empirical adjustment coefficients. The dynamic viscosities of the liquid mixtures have been calculated using several empirical relations due to Hind, Grunberg and Nissan, Katti and Chaudhri, Tamura &Kurata, from graph 2 shows the relative applicability with standard deviation(σ) of viscosity for liquid mixture of acetone with 2-propanol at temperature of 303.15K.

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Table 03 Viscosity theories of acetone with 2-propanol at 303.15K temperatures

Temperature		Hind (H_{12})	Grunberg & Nissan (G_{12})	Katti&chawdhary (W_{vis})	Tamura& Kurata(T_{12})
303.15 K	Interaction parameter	-1.1276	-0.9084	-0.8682	19.6800
	Standard deviation(σ)	2.1846	1.2483	3.5711	0.9229

It is clear that Tamura & Kurata theory could not give accurate values compared to experimental values. These theories generally fail to predict accurately the values where strong interactions are supposed to exist due to the limitations and approximations incorporated in these theories. Various interaction parameters and their corresponding standard deviations of viscosity computed from different theories in liquid mixture of acetone with 2-propanol at temperature of 303.15k. All the empirical models gave a reasonable fit in all these mixture. The Grunberg and Nissan is in good agreement with the experimental values by the evidence of the interaction parameter and standard deviation .The estimated standard deviations are smaller in all cases indicating that the present mixture viscosities are well correlated by these viscosity models.

Graphs for Variation of Speed of sound theories from figure 1 and the viscosity theories from figure 2 with respect to whole range of mole fraction(X_1) at 303.15K temperature for acetone + 2-propanol binary system

Fig 01

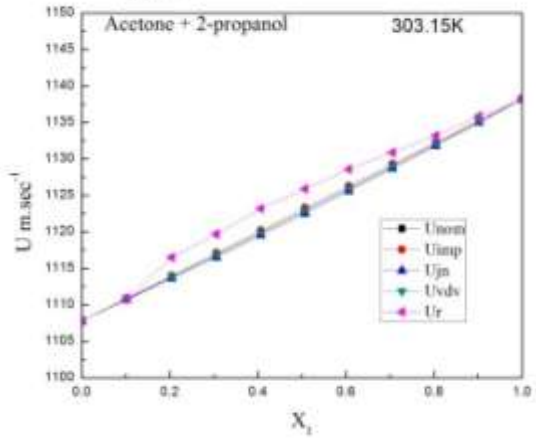

Fig 02

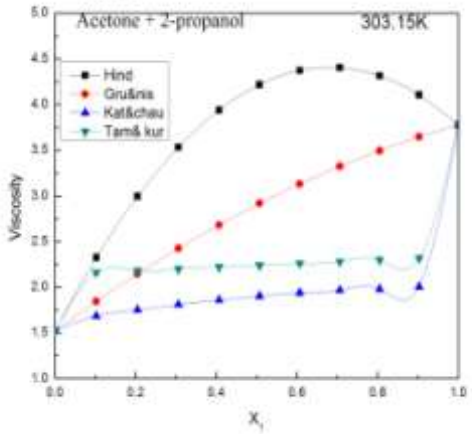

Fig 01 variation of speed of sound theories w.r.to mole fraction at 303.15K temp

Fig 02 variation of viscosity theories w.r.to mole fraction at 303.15K temp

Thus, the observed deviation of theoretical values of speed of sound from the experimental values shows that the molecular interaction is taking place between the unlike molecules in the liquid mixtures. Hence the observed deviation shows that the molecular interaction is taking place between the unlike molecules in the liquid mixture. This suggests the existence of strong tendency for the association between component molecules as a result of Hydrogen bonding.

V. Conclusions

The observed deviation of theoretical values of viscosity and speed of sound from the experimental values is attributed to the presence of intermolecular interactions.The computed speed of sound and viscosity

values from different theories have been correlated with the experimentally measured values. Speed of sound values obtained from Nomoto's and Junjie's method relations are in good agreement with the experimental values. It may be concluded that out of these theories, The APE and Chi square values also support this theory. The experimental viscosity values are also compared with the viscosity values obtained from different empirical relations and the Grunberg and Nissan is in good agreement with the experimental values .The interaction parameter and standard deviation also supports this conclusion.

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