International Journal of Science, Environment
and Technology, Vol. 2, No 3, 2013, 502 –509

ISSN 2278-3687 (O)

THEORETICAL PREDICTION OF SPEEDS OF SOUND FOR BINARY MIXTURES OF 2-METHYL-1-PROPANOL WITH N-ALKANES AT 298.15 K

Gyan Prakash Dubey[*] and Monika Sharma
Department of Chemistry, Kurukshetra University, Kurukshetra 136119, India
E-mail: drgyandubey@gmail.com (**Corresponding Author*)

Abstract: Different empirical and semi empirical relations to calculate speed of sound namely Nomoto's relation, Van Deal's ideal mixing relation, impedance dependence relation, Junjie's relation, Jacobson's free length theory and Schaaff's collision factor theory have been applied on three binary liquid mixtures. The experimental and calculated speeds of sound of binary mixtures of 2-methyl-1-propanol with n-hexane, n-octane and n-decane at 298.15 K and atmospheric pressure are compared. To examine the relative merits of these theories and relations, the results are discussed in terms of standard percentage deviations.

Keywords: Speed of sound, density, empirical relations, standard percentage deviation.

1. Introduction

Speed of sound has been a subject of active interest during the recent past. Attempts have been made to show the significance of thermodynamic properties derived from speed of sound and related data with intermolecular interactions in binary liquid mixtures [1, 2]. The present paper is part of our systematic studies on thermodynamic properties for binary mixtures of alcohols and alkanes which have great interest in several chemical industries. In the present paper we have reported the density and speed of sound for binary mixtures of alcohols and alkanes which have great interest in several chemical industries. Herein, we report the measurements of densities (ρ) and speeds of sound (u) of 2-methyl-1-propanol, $(CH_3)_2CHCH_2OH$ with *n*-hexane, C_6H_{14}, *n*-octane, C_8H_{18} and *n*-decane, $C_{10}H_{22}$ over the entire composition range at 298.15 K and atmospheric pressure. Furthermore, using the experimental results, theoretical estimation of the speed of sound using Nomoto's relation (NR), Van Deal ideal mixing relation (IMR), impedance dependence relation (IDR), Junjie's relation (JR), Jacobson's free length theory (FLT) and Schaaffs' collision factor theory (CFT) has been done for these binary mixtures.

*Received May 3, 2013 * Published June 2, 2013 * www.ijset.net*

2. Experimental

Densities of these mixtures were measured by using a bicapillary pycnometer whereas for the measurements of speeds of sound a crystal controlled variable path ultrasonic interferometer (model F-81, supplied by Mittal Enterprises, New Delhi) was used. The experimental densities and speeds of sound of the pure components at 298.15 K are summarized in Table 1. Details of purification of materials, experimental procedure and calibration of apparatus / instruments are given elsewhere [1].

3. Results and discussion

The values of density and speed of sound of all binary mixtures at 298.15 K are reported in table 2. The following empirical and semi-empirical relations were used for theoretical estimation of speed of sound in the studied binary mixtures [3-9]:

(i) Nomoto's relation (NOM) which is based on the assumption of the additivity of molar sound velocity and no volume change on mixing is given as

$$u=[\,(x_1R_1+x_2R_2)\,/\,(x_1V_1^*+x_2V_2^*)\,]^3 \qquad (1)$$

where x_1, R_i and V_i^* are mole fraction, molar speed of sound and molar volume of ith component respectively and R_i is given by

$$R_i=(M_i\,u_i^{1/3})/\rho_i^* \qquad (2)$$

where M_i, u_i and ρ_i^* are molecular weight, speed of sound and density of ith component respectively.

(ii) Van Deal ideal mixing relation (IMR):

$$(\,\sum x_i\,M_i)^{-1}\times(\,u^2)^{-1}=\sum(\,x_i\,/\,M_i\,u_i^2\,) \qquad (3)$$

where x_i and M_i are mole fraction and molar mass of ith component respectively.

(iii) Impedance dependence (ID) relation:

$$u=\sum(\,x_i\,Z_i\,)\,/\sum(\,x_i\,\rho_i^*\,) \qquad (4)$$

where $Z_i=u_i\,\rho_i^*$ is specific acoustic impedance of component *i*.

(iv) Zhang–Junjie has obtained the following relation (JR) for the measurement of speed of sound in binary liquid mixtures:

$$u=\sum(\,x_i\,V_i^*\,)\,/\,(\,\sum(\,x_iM_i\,)^{1/2}\,)\times\left[\,\sum(\,x_i\,V_i^*\,/\,\rho_i\,u_i^2\,)\,\right]^{1/2} \qquad (5)$$

(v) Jacobson's free length theory (FLT) expresses the speed of sound by the following relation:

$$u = K / L_f \, \rho^{1/2} \tag{6}$$

where K is the Jacobson's constant and it is temperature dependent. L_f is the intermolecular free length and ρ is density of the mixture. The L_f is obtained by

$$L_f = (V_m - \sum x_i V_{0i}) / \sum (x_i Y_i) \tag{7}$$

where $V_{0\,i}$ is the molar volume of the pure component i at absolute zero and it given by Sugden's formula:

$$V_{0i} = V_i^* \left[(1 - T) / T_{c,i} \right]^{0.3} \tag{8}$$

where $T_{c,\,i}$ is the critical temperature and $Y_i = (36\,\pi\,N\,V_{0\,i}^2)^{1/3}$ is the surface area per mole for the pure component i. The values of critical temperature for the pure components at 298.15 K have been taken from literature [10].

(vi) Schaaff's collision factor theory (CFT):

$$u = u_\infty \left[(\sum x_i S_i) \times (\sum x_i B_i) \right] / V_m \tag{9}$$

where $S = [(u\,V) / (B\,u_\infty)]$ and $B = [(4/3)\,\pi\,r_m^3]$ represent collision factor and geometrical volume respectively, u_∞ is taken as constant value of 1600 $\mathrm{ms^{-1}}$. $r_m = [(3\,b/16\,\pi\,N)^{1/3}]$ stands for molecular radii and b is van der Waal's constant which is given as

$$b = (M/\rho) - (RT/\rho^2 u^2)\,[\{1 + (M u^2 / 3RT)\}^{1/2} - 1] \tag{10}$$

In order to perform a numerical comparison of the estimation capability of the various empirical and semiempirical formulae used to predict speed of sound in pure liquids and liquid mixtures, we have calculated the standard percentage deviations $(\sigma\,\%)$ using the relation:

$$\sigma\,\% = [\,\sum \{\,100\,(\text{exptl.} - \text{theo.})/\text{exptl.}\}^2 / (n-1)]^{1/2} \tag{11}$$

where n represents the number of experimental data points.

The experimental and calculated speeds of sound of binary mixtures of $(CH_3)_2CHCH_2OH$ with C_6H_{14}, C_8H_{18} and $C_{10}H_{22}$ at 298.15 K are graphically presented in Figures 1-3. To examine the relative merits of these theories and relations, standard percentage deviations ($\sigma\,\%$) are calculated and represented as a bar diagram in Figure 4.

A close look at Figure 4 shows that for $(CH_3)_2CHCH_2OH$ + C_6H_{14} [system (I)] minimum $\sigma\%$ is observed in the case of JR, followed by NR, CFT, IMR, ID and FLT. For $(CH_3)_2CHCH_2OH$ + C_8H_{16} [system (II)], IMR predicts the data with minimum $\sigma\%$ followed by CFT, JR, NR, ID, FLT while for $(CH_3)_2CHCH_2OH$ + $C_{10}H_{22}$ [system (III)], CFT predicts the estimation of speed of sound with minimum $\sigma\%$, followed by ID, JR, NR, IMR, FLT. Thus it is found that the speeds of sound evaluated using various empirical and semiempirical formulas are satisfactory to different extents in different mixtures. It is observed that out of all the relations discussed above, deviations obtained by FLT are quite large and in the present case this theory does not yield satisfactory results. This is in good agreement with the conclusions drawn by others [11,12] that large deviations from FLT are observed for mixtures containing self-associated liquid(s), as alkanol in the present systems. The slight discrepancy in the values obtained from CFT can be ascribed to the fact that in CFT; the molecules are treated as real, non-elastic spheres [13,14]. The deviations in the speeds of sound evaluated using IMR from experimental values can be attributed to the non-ideal nature of the mixture. It is also evident from Figure 4 that in spite of being empirical, the Junjie's relation (JR) performs well in the studied systems.

References

[1] G P Dubey, M Sharma, J Chem. Eng. Data 2007, 52, 449.

[2] G P Dubey, M Sharma, S L Oswal, J. Chem. Thermodyn. 2009, 41, 849.

[3] O. Nomoto, J. Phys. Soc. Jpn. 1958, 13, 1528.

[4] W. Van deal, *Thermodynamic Properties and Velocity of Sound*, Butterworth, London 1975.

[5] F. N. Tasi, J. Chem. Eng. Data 1994, 39, 441.

[6] Z. Junjie, J. Chem. Univ. Sci. Tech. 1984, 14, 298.

[7] B. Jacobson, Acta Chem. Scand. A. 1952, 8, 1485.

[8] W. Schaffs, Landolt-Bronstein *Numerical Data and Functional Relationships in Science and Technology*, Group II, Vol. 5, (Molecular Acoustics). K.-H. Hellwege ed., Springer-Verlag, Berlin 1967.

[9] W. Schaaffs, Acoustica 1975, 33, 272.

[10] J. A Riddick, W. B. Bunger, T. K. Sakano, *Organic solvents, Physical properties and methods of purifications* 4th ed., Wiley-interscience, New York 1986.

[11] B. Jacobson, Acta Chem. Scand. 1951, 5, 1214; 1952, 6, 1485.

[12] J. D. Pandey, R. Dey, D. K. Dwivedi, Pramana 1999, 52, 187.

[13] W. Schaaffs, Z. Phys. 1939, 114, 110.

[14] W. Schaaffs, Z. Phys. 1940, 115, 69.

[15] K. N. Marsh, *TRC Data Bases for Chemistry and Engineering–TRC Thermodynamic Tables*; Texas A & M University, College Station, TX 1995.

[16] M. F. Bolotnikov, Y. A. Neruchev, Y. F. Melikhov, V. N. Verveyko, M. V. Verveyko, J. Chem. Eng. Data 2005, 50, 1095.

[17] D. Missopolinuo, I. Tsivintzelis, C. Panayiotou, Fluid Phase Equilib. 2006, 245, 89.

[18] A. Touriño, L. M. Casás, G. Marino, M. Iglesias, B. Orge, J. Tojo, Fluid Phase Equilib. 2003, 206, 61.

[19] *TRC Thermodynamic Tables; Hydrocarbons*; Thermodynamics Research Center, The Texas A & M University System, College Station, Texas 1998.

[20] T. M. Aminabhavi, M. I. Aralaguppi, S. B. Harogoppad, R. H. Balundgi, J. Chem. Eng. Data 1993, 38, 31.

[21] E. Langa, A. M. Marinar, J. I. Pardo, J. S. Urieta, J. Chem. Eng. Data 2007, 52, 1228.

[22] T. Khasanshin, A. Shchemelev, High Temp. 2001, 39, 60.

[23] G. Savaroglu, E. Aral, Pramana 2006, 66, 435.

[24] J. M. Resa, C. Gonzalez, J. M. Goenaga, M. Iglesias, Phys. Chem. Liq. 2005, 43, 65.

[25] E. Junquera, G. Tardajos, E. Aicart, J. Chem. Thermodyn. 1998, 20, 1461.

[26] M. M. Pineiro, E. Mascato, L. Mosteiro, J. L. Legido, J. Chem. Eng. Data 2003, 48, 758.

Table 1

Experimental and literature values of densities (ρ^*) and speeds of sound (u^*) of pure liquid components at 298.15 K and atmospheric pressure

Components	$\rho^* \times 10^{-3}$ (kg m^{-3})		u^* (m s^{-1})	
	Exptl.	Lit.	Exptl.	Lit.
C_6H_{14}	0.6549	0.65489 [15]	1078.5	1078.1 [22]
		0.65493 [16]		1078 [23]
		0.65484 [10,17]		1076 [16]
C_8H_{18}	0.6986	0.69862 [10]	1170.9	1169.6 [24]

		0.69851 [17]		1172.02 [25]
$C_{10}H_{22}$	0.7259	0.72635 [10]	1235.4	1234.7 [26]
		0.7261 [18]		1234.75 [18]
		0.72614 [19]		
$(CH_3)_2CHCH_2OH$	0.7982	0.7982 [10,20]	1191.4	1191 [20]
		0.7978 [10,19]		1188 [21]
		0.79803 [21]		

Table 2

Densities (ρ) and speeds of sound (u) for binary mixtures of x_1 $(CH_3)_2CHCH_2OH$ with C_6H_{14}, C_8H_{18} and $C_{10}H_{22}$ at 298.15 K

x_1	$\rho\times10^{-3}$ (kg m^{-3})	u (m s^{-1})	x_1	$\rho\times10^{-3}$ (kg m^{-3})	u (m s^{-1})	x_1	$\rho\times10^{-3}$ (kg m^{-3})	u (m s^{-1})
	$(1-x_1)C_6H_{14}$			$(1-x_1)C_8H_{18}$			$(1-x_1)C_{10}H_{22}$	
0.0554	0.6601	1077.5	0.0589	0.7015	1168.3	0.0728	0.7281	1228.7
0.1040	0.6649	1077.5	0.1165	0.7045	1166.5	0.1021	0.7290	1226.6
0.2000	0.6751	1080.1	0.2050	0.7098	1164.8	0.2032	0.7326	1219.9
0.3274	0.6901	1086.7	0.2792	0.7147	1164.0	0.2976	0.7364	1215.2
0.4173	0.7016	1094.1	0.3371	0.7189	1163.1	0.3547	0.7390	1212.2
0.4666	0.7083	1099.2	0.4081	0.7246	1162.7	0.4171	0.7421	1209.4
0.5057	0.7138	1103.5	0.4662	0.7296	1163.3	0.5016	0.7470	1206.1
0.5589	0.7215	1110.0	0.5126	0.7339	1163.7	0.6084	0.7542	1201.8
0.6090	0.7290	1116.9	0.6126	0.7441	1166.3	0.6575	0.7580	1200.2
0.7073	0.7446	1132.5	0.6615	0.7495	1168.4	0.7027	0.7619	1198.4
0.8051	0.7612	1150.0	0.7069	0.7549	1170.1	0.8004	0.7716	1195.1
0.8610	0.7712	1161.3	0.7855	0.7650	1173.6	0.8952	0.7829	1192.9
0.9149	0.7813	1172.5	0.8615	0.7758	1178.6	0.9497	0.7905	1192.0
0.9376	0.7857	1177.5	0.9523	0.7901	1187.0	0.9848	0.7958	1191.8

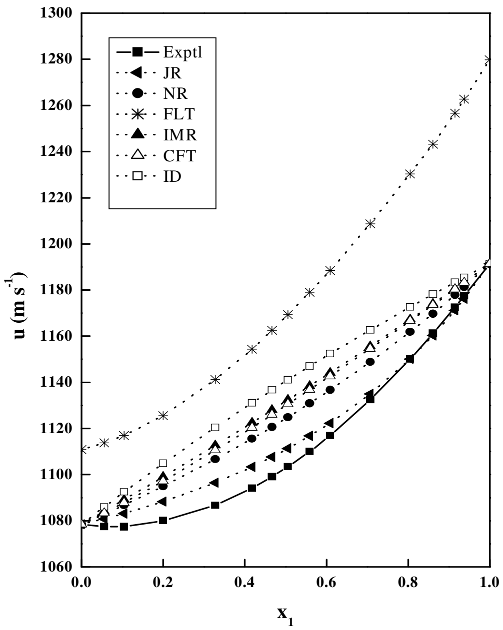

Figure 1. Experimental and theoretically evaluated speeds of sound (u) for the binary mixtures of $(CH_3)_2CHCH_2OH(1) + C_6H_{14}(2)$ at 298.15 K

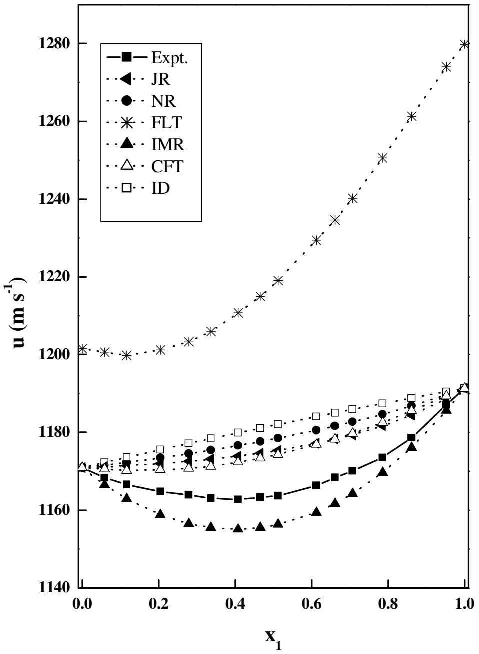

Figure 2. Experimental and theoretically evaluated speeds of sound (u) for the binary mixtures of $(CH_3)_2CHCH_2OH$ (1) + C_8H_{18} (2) at 298.15 K

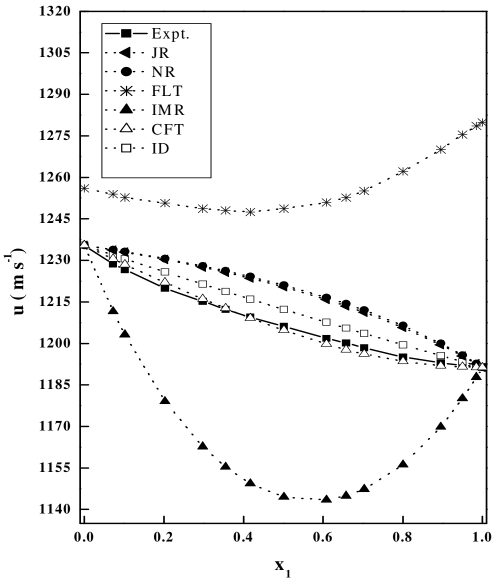

Figure 3. Experimental and theoretically evaluated speeds of sound (u) for the binary mixtures of $(CH_3)_2CHCH_2OH$ (1) + $C_{10}H_{22}$ (2) at 298.15 K

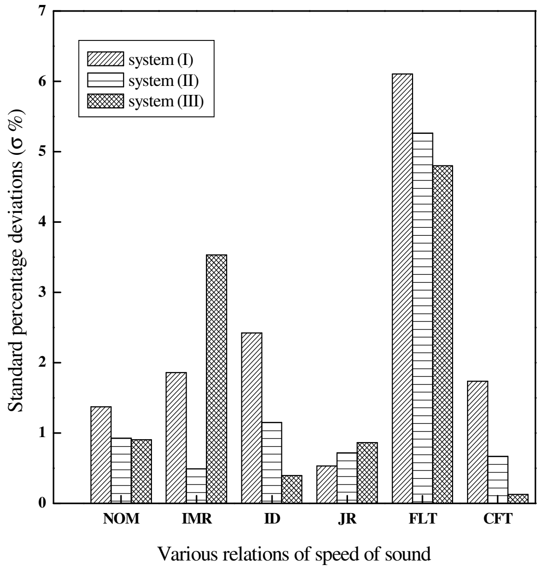

Figure 4. Standard percentage deviations (σ %) for the mixtures of $(CH_3)_2CHCH_2OH$ + C_6H_{14} (I); $(CH_3)_2CHCH_2OH$ + C_8H_{18} (II); and $(CH_3)_2CHCH_2OH$ + $C_{10}H_{22}$ (III) at 298.15 K.