

Speed of Sound, Isentropic Compressibility and Acoustic Impedance for Long Chain Non-polar Molecule with Isomeric Alcohols at T=288.15 to 318.15 K

Arun K. Singh, Ashish Singh, Sandeep Singh and Gyan Prakash

Abstract-Theoretical results for sound speed, isentropic compressibility, and acoustic impedance for two binary systems, 1-Butanol + n-Dodecane and 2-Butanol + n-Dodecane, were derived from Peleteiro et al's measurements at temperatures of 288.15, 298.15, 308.15, 318.15 K and atmospheric pressure over the entire composition range. The mixing properties and interactions of these liquids were explored using the Flory model, the Ramaswamy and Anbananthan (RS) model, and the Glinski model. The Redlich-Kister polynomial equation was used to fit deviations in the speed of sound (u). In addition, the McAllister multi-

body interaction model is applied. The molecular interactions from these liquid state models were explored and connected with the features of the liquids. Finally, it was discovered that when compared to related models, the McAllister multibody interaction model (non-associated) produces good results, whereas the Flory model produces greater deviations.

Index Terms: -Speed of sound, isentropic compressibility, acoustic impedance, molecular interactions, binary liquid mixtures, liquid state models

1. INTRODUCTION

The goal of the research was to use associated and non-associated models to investigate the behaviour of binary liquid mixtures and their molecular interactions. We present the theoretical results of sound speed, isentropic compressibility, and acoustic impedance for two binary liquid mixtures, namely 1-Butanol + n-Dodecane and 2-Butanol + n-Dodecane at temperatures 288.15, 298.15, 308.15, and 318.15 K and atmospheric pressure over the entire composition, based on Peleteiro et al's [1] measured work. Dodecane, a liquid alkane hydrocarbon, is used in reprocessing plants as a solvent, distillation chaser, scintillator component, and diluents for tributyl phosphate [2]. Other traditional aviation fuels, such as n-dodecane, have been employed in recent years. 1-Butanol is employed as a solvent in a range of chemical and textile processes, as well as a chemical intermediate, a paint thinner and a solvent in other coating applications, and as a basis for perfumes.

As a swelling agent in textiles, a segment of hydraulic break fluids [5], cleaning details, degreasers, and anti-agents [6], and a segment of metal flotation agents [7] and wood-treating frameworks [8], n-butanol is used in a variety of ways. Butanol is a potential bio-fuel that can be utilized in cars that are meant to run on gasoline [9]. 2-Butanol is a flammable secondary alcohol that is totally miscible with polar organic solvents like ethers and other alcohols. It's a major industrial solvent that's present in a variety of household cleaners and paint removers, and it's also employed in small amounts as scents or artificial flavours. Sound velocity can be used to investigate the thermodynamic characteristics and molecular interactions of liquids and liquid mixtures [10-13]. Many researchers [14-16] have done extensive effort in the past to examine the interactions and molecular behaviour of sound velocity and to correlate it with other physical and thermodynamic characteristics. Based on Eyring's theory of absolute reaction rates, the data were examined using the Ramaswamy and Anbananthan (RS) model [17], the Flory model [19], and the McAllister multi body interactive model [20]. The first two models, the RS and the Glinski model (associated), use the association constant as an adjustable parameter, whereas Flory and others (non-associated) use liquid additivity. We choose liquids with long carbon chains (non-polar) and butanol isomer (polar) molecules for this purpose. Deviations in ultrasonic velocity, u were determined from these results and fitted to the Redlich-Kister polynomial equation [21]

Manuscript revised on August 31, 2023 and published on September 30, 2023

Arun K. Singh, Associate Professor Department of Chemistry, Bhawan Mehta Mahavidyalaya, Bharwari, Kaushambi-212201, India. Email-akumar13april@gmail.com

Ashish Singh, Department of Chemistry, VSSD College, Kanpur-208002, India

Sandeep Singh, Department of Chemistry, VSSD College, Kanpur-208002, India

Gyan Prakash, Associate Professor Department of Chemistry, VSSD College, Kanpur-208002, India. (Corresponding author)
Email- gyanprakashvssd1921@gmail.com

to get binary coefficients and standard errors. Because of the interaction of long chain carbon molecules with

butanol isomer, the mixing behaviours of such liquid combinations are intriguing.

2.MODELS

2.1 Flory model

By using the cell partition function and a simple van der Waals energy-volume relation in the Prigogine cell model [22], Flory and collaborators were able to obtain the equations for the mixing functions by choosing the m,n potential. Patterson et al [24] defined a close relationship between the Flory theory and the corresponding state theory of Prigogine [23] by using a basic cell model for spherical chain molecules in the form of reduction parameters.

Eq. takes the form; with the particular (3, ∞) choice of m,n potential

$$\tilde{\sigma}(\tilde{v}) = [M \tilde{v}^{-5/3} - (\frac{\tilde{v}^{1/3} - 1.0}{\tilde{v}^2}) \ln(\frac{\tilde{v}^{1/3} - 0.5}{\tilde{v}^{1/3} - 1.0})] \quad (1)$$

As a result, the surface tension of a liquid combination

can be calculated using the following formula:

$$\sigma = \sigma^* \tilde{\sigma}(\tilde{v}) \quad (2)$$

The empirical relationship of Auerbach [25] relates surface tension to acoustic velocity as follows:

$$u_{Flory} = \left(\frac{\sigma}{6.3 \times 10^{-4} \rho} \right)^{2/3} \quad (3)$$

Patterson and Rastogi [26] utilized the following reduction parameters to expand the related state theory to deal with surface tension:

$$\sigma^* = k^{1/3} P^{*2/3} T^{*1/3} \quad (4)$$

The liquid's characteristic surface tension is referred to as this. The Boltzmann constant, k, is used here. While transitioning from the bulk to the surface phase, a segment experiences an increase in configurational energy equal to $-M \tilde{U}(\tilde{v})$ due to the loss of a fraction, M, of its nearest neighbours at the surface. Its most appropriate value is between 0.25 and 0.29.

From the resultant partition function, Flory deduced the simplified equation of state as,

$$\frac{\tilde{P} \tilde{v}}{\tilde{T}} = \frac{\tilde{v}^{1/3}}{\tilde{v} - 1} - \frac{1}{\tilde{v} \tilde{T}} \quad (5)$$

The reduced quantities \tilde{v} , \tilde{P} and \tilde{T} are given by,

$$\tilde{P} = \frac{P}{P^*} = \frac{2PV^*}{S\eta}, \quad \tilde{T} = \frac{T}{T^*} = \frac{2V^* cKT}{S\eta} \quad \text{and} \\ \tilde{v} = \frac{V}{V^*} = \frac{V}{V^*} \quad (6)$$

The reduced molar volume and characteristic pressure are calculated using eq.(6) as follows: $\tilde{v} = [\frac{\alpha T}{(3+3\alpha T)} + 1]^3$

$$P^* = \frac{\alpha}{\beta_T} T \tilde{v}^{-2} = \gamma T \tilde{v}^{-2} \quad (7)$$

where k_T and γ are the isothermal compressibility and thermal pressure coefficients, respectively, and α is the thermal expansion coefficient at p=0. According to eqs. (6) and (7), the numbers T^* , P^* , and V^* can be determined from, T, and V. (7).

The equations for characteristic pressure and decreased temperature of mixture were developed by Pandey et al. [26].

$$\tilde{T} = T/T^* = \frac{T}{P^* / (\frac{\psi_1 P_1^*}{T_1^*} + \frac{\psi_2 P_2^*}{T_2^*})} \quad (8)$$

where P^* is the binary system's characteristic pressure and can be written as

$$P^* = [\psi_1 P_1^* + \psi_2 P_2^* - (\psi_1 \theta_2 X_{12} + \psi_2 \theta_1 X_{21})] \quad (9)$$

Here, x_{12} , x_{21} are the interaction parameters, which were calculated using the following equations and the well-known Berthelot connection, $\eta_{ij} = (\eta_{ii} \eta_{jj})^{1/2}$. All of the symbols used in the equations above have their typical meanings, as explained by Flory.

2.2 RS Model

Ramswamy and Anbanathan postulated that when a solute is added to the solvent and the acoustic impedance is linear with the mole fraction of components, the molecules interact according to the equilibrium as:



and the association constant K_{as} may be defined as;

$$K_{as} = \frac{[AB]}{[A][B]} \quad (11)$$

where [A] is the amount of solvent in the liquid mixture and [B] is the amount of solute. When we combine the linearity constraint with composition, we get

$$u_{obs} = x_A u_A + x_{AB} u_{AB} \quad (12)$$

where x_A , x_{AB} , u_A , u_{AB} , and u_{obs} are the mole fraction of A, associate AB's mole fraction, speed of sound of A, associate AB's speed of sound, and observed speed of sound, respectively. The equilibrium reaction in eq. (12)

is erroneous because there are molecules of non-related component in the liquid mixture along with the linked components. When a non-associated component is present in a liquid mixture, eq has the following form:

$$\sigma_{obs} = [x_A u_A + x_B u_B + x_{AB} u_{AB}] \quad (13)$$

where x_B and u_B are B 's mole fraction and sound speed, respectively (non-associated component). The equilibrium concentration of the pure associate AB can be calculated as follows:

$$K_{as} = \frac{[AB]}{(C_A - [AB])(C_B - [AB])} \quad (14)$$

The starting molar concentrations of the components A and B are C_A and C_B , respectively. Any value of K_{as} can be used to compute the equilibrium value of $[AB]$ for any mixture composition, as well as $[A] = C_A - [AB]$ and $[B] = C_B - [AB]$. Equation (14) becomes, when molar concentration is replaced by activities.

$$K_{as} = \frac{a_{AB}}{(a_A - a_{AB})(a_B - a_{AB})} \quad (15)$$

where a_A , a_B , and a_{AB} denote component A , component B , and association AB , respectively. The value of K_{as} can be calculated using eq (15) as follows:

$$K_{as} = \frac{a_{AB}}{a_A a_B - a_A a_{AB} - a_B a_{AB} + a_{AB}^2} \quad (16)$$

It is feasible to compare the speed of sound estimated using eq. (13) with the experimental values, assuming any value of speed of sound in the hypothetical pure component. By gradually altering both the adjustable parameters K_{as} and AB , different values of the sum of squares of deviations can be obtained, such as;

$$S = \sum (u_{obs} - u_{cal})^2 \quad (17)$$

The observed and calculated sound speeds are denoted by u_{obs} and u_{cal} , respectively. With the values of K_{as} and u_{AB} , the least value of S is adjusted. In certain circumstances, the value of S is large and fluctuates quickly, whereas in others, it is low and moves slowly. We changed the value of u_{AB} so that it was neither lower than the least measured sound speed nor considerably higher than the greatest.

2.3 Model Suggested by Glinski

Glinski[18] assumed additivity with the volume percent, of the components to improve the results, which is similar to the improved version of Natta and Baccaredda model [27]

$$as, u_{cal} = \frac{u_A u_B u_{AB}}{\phi_A u_B u_{AB} + \phi_B u_A u_{AB} + \phi_{AB} u_A u_B} \quad (18)$$

where u_{cal} is the theoretical sound speed of a binary liquid mixture, A , B are the volume percentages of component A and B , and u_A , u_B , and u_{AB} are the sound

speeds of components A , B , and AB , respectively. Similar to the RS model, the numerical approach and determination of the association constant, K_{as} , were used. The advantage of this method over the previous one was that it did not require any data on liquid mixture densities other than those of pure components needed to calculate volume fractions. Reis et al [28] and others [29] developed and expanded on the significance of related liquids previously described.

2.4 McAllister – three body model

Eyring [30] proposed the following formula for kinematic viscosity of a liquid and its relationship to temperature:

$$\partial = \frac{hN}{M} e^{\Delta G^*/RT} \quad (19)$$

where ∂ , h, N , M , $R T$ and ΔG^* are kinematic viscosity, plank constant, molar mass, gas constant absolute temperature and free energy of activation respectively. The development of the particle between two layers of fluid might be viewed as the section of the framework over a potential energy barrier, identified with ΔG^* .

McAllister followed Eyring's lead and looked at different three-bodied planar encounters in molecules of type (1) and (2), recommending that the absolute free energy of enactment is determined by the free energy of initiation (G_i , G_{ij} , or G_{sijk}) of individual collaborations and their division of complete events as;

$$(x_i^3, x_i^2 x_j, x_j^2, x_i x_j^2 \text{ or } x_i x_j x_k) \\ \Delta G^* = x_1^2 \Delta G_1^* + x_1^2 x_2 \Delta G_{121}^* + 2x_1^2 x_2 \Delta G_{112}^* + x_1 x_2^2 \Delta G_{212}^* \\ + 2x_1 x_2^2 \Delta G_{123}^* + x_2^3 \Delta G_2^* \quad (20)$$

Using the following assumptions as a starting point:

$$\Delta G_{121}^* = \Delta G_{112}^* \equiv \Delta G_{12}^* \text{ and}$$

$$\Delta G_{121}^* = \Delta G_{122}^* = \Delta G_{21}^*$$

Also,

$$\Delta G_{12}^* = \frac{\Delta G_{121}^* + 2\Delta G_{112}^*}{3} \text{ and}$$

$$\Delta G_{21}^* = \frac{\Delta G_{212}^* + 2\Delta G_{122}^*}{3} \quad (21)$$

As a result, eq.(24) can be expressed as;

$$\Delta G^* = x_1^3 \Delta G_1^* + 3x_1^2 x_2 \Delta G_{12}^* + 3x_1 x_2^2 \Delta G_{21}^* + x_2^3 \Delta G_2^* \quad (22)$$

Using eq. (20) for each set of interactions (i.e. 111,121,211, 112; 212, 122, 221and 222), the following equation is obtained:

$$\ln u = x_1^3 \ln u_1 + 3x_1^2 x_2 \ln u_{12} + 3x_1 x_2 \ln u_{21} \\ + x_2^3 \ln u_2 - \ln[x_1 + x_2 M_2 / M_1] + 3x_1^2 x_2 \ln[(2 + M_2 / M_1) / 3]$$

$$+ 3x_1 x_2^2 \ln[(1 + 2M_2 / M_1) / 3] + x_2^3 \ln[M_2 / M_1] \quad (23)$$

here, $M_{12} = \frac{2M_1 + M_2}{3}$ and

$$M_{21} = \frac{M_1 + 2M_2}{3} \quad (24)$$

2.5 McAllister –four body model

If molecules have a large size difference, and we consider multiple partnerships and their proportion of absolute events, the energy of enactment activation could be made up of the energy of initiations of numerous collaborations.

$$\Delta G^* = x_1^4 \Delta G_1^* + 4x_1^3 x_2 \Delta G_{112}^* + 6x_1^2 x_2^2 \Delta G_{112}^* + 4x_1 x_2^3 \Delta G_{222}^* + x_2^4 \Delta G_2^* \quad (25)$$

Following the same technique as before, the following equation for four-body interaction is obtained:

$$\begin{aligned} \ln u_{mix} = & x_1^4 \ln u_1 + 4x_1^3 x_2 \ln u_{1112} + 6x_1^2 x_2^2 \ln u_{1122} \\ & + 4x_1 x_2^3 \ln u_{222} + x_2^4 \ln u_2 - \ln(x_1 + x_2 M_2 / M_1) \\ & + 4x_1^3 x_2 \ln[(3 + M_2 / M_1) / 4] + 6x_1^2 x_2^2 \ln[(1 + M_2 M_1) / 2] \\ & + 4x_1 x_2^3 \ln[(1 + 3M_2 / M_1) / 4] + x_2^4 \ln(M_2 / M_1) \end{aligned} \quad (26)$$

where u , x_i , u_i , M_1 , x_2 , u_2 , and M_2 represent the mixture's surface tension, mole fraction, sound speed, and

molecular weight of pure components 1 and 2, respectively.

3. RESULTS & DISCUSSION

The literature [1] was used to obtain experimental density and sound speed data for pure liquids at various temperatures. Panday et al [31] provided the thermal expansion coefficients (α) and isothermal compressibility coefficients (k_T). The Redlich-Kister equation can be used to calculate sound velocity deviations (u).

$$y = x_i (1 - x_1) \sum_{i=0}^p A_i (2x_1 - 1)^i \quad (27)$$

where y denotes the sound velocity deviation (u), x_i denotes the mole fraction, and A_i denotes the coefficient. Multiple regression analysis using the least squares approach was used to calculate the coefficient values, which are given along with the standard deviations between the experimental and fitted values of the corresponding function (Table 1). The standard deviation (σ) range for sound velocity was 0.23 - 0.54, with the greatest value obtained at 288.15 K for the 1-butanol+dodecane mixture.

Table 1 Coefficient of Redlich- Kister and standard deviation for speed of sound of binary liquid mixtures.

T/K	1-Butanol+n-Dodecane					2-Butanol+n-Dodecane				
	A ₀	A ₁	A ₂	A ₃	$\Delta\delta$	A ₀	A ₁	A ₂	A ₃	$\Delta\delta$
288.15	-5.95	-2.26	-26.04	18.01	0.53	-6.78	0.86	-9.59	15.21	0.38
298.15	-14.41	-3.14	-26.22	14.54	0.45	-14.62	-6.63	-15.15	17.80	0.36
308.15	-22.89	-5.27	-26.97	13.79	0.40	-20.94	-12.52	-21.72	18.11	0.32
318.15	-31.39	-5.20	-22.78	2.65	0.23	-25.24	-15.15	-25.89	10.67	0.24

Table 2. Parameters of McAllister-3 and 4 Body interaction coefficients and their standard deviations ($\Delta\delta$) for speed of sound of binary liquid mixture.

T/K	McAllister three Body Model			McAllister four Body Model			
	A	B	$\Delta\delta$	A	B	C	$\Delta\delta$
1-Butanol+N-Dodecane							
288.15	709.10	969.36	0.74	1334.02	1322.44	1315.44	0.31
298.15	687.34	939.90	0.68	1294.01	1282.65	1275.35	0.30
308.15	665.82	910.90	0.60	1254.29	1243.67	1235.75	0.30
318.15	644.36	882.82	0.54	1215.21	1204.58	1197.64	0.24
2- Butanol+n-Dodecane							
288.15	700.07	963.29	1.17	1317.00	1305.02	1311.26	0.44
298.15	676.84	934.35	0.97	1273.27	1266.25	1270.66	0.48
308.15	653.99	905.78	0.74	1229.76	1228.48	1230.41	0.48
318.15	631.55	877.78	0.52	1187.17	1190.67	1191.28	1.79

Table 3. Parameters of McAllister-3 and 4 body interaction coefficients and their standard deviations ($\Delta\delta$) for acoustic impedance of binary liquid mixture.

McAllister three Body Model/				McAllister four Body Model			
1-Butanol+N-Dodecane							
T/K	A	B	$\Delta\delta$	A	B	C	$\Delta\delta$
288.15	0.5419	0.7378	0.0003	1.0308	1.0165	0.9936	0.0003
298.15	0.5201	0.7082	0.0003	0.9902	0.9761	0.9538	0.0003
308.15	0.4989	0.6792	0.0003	0.9504	0.9367	0.9148	0.0003
318.15	0.4778	0.6513	0.0003	0.9113	0.8979	0.8773	0.0002
2- Butanol+n-Dodecane							
288.15	0.5335	0.7310	0.0004	1.0152	0.9990	0.9894	0.0004
298.15	0.5102	0.7018	0.0004	0.9707	0.9600	0.9488	0.0004
308.15	0.4874	0.6732	0.0005	0.9267	0.9221	0.9088	0.0004
318.15	0.4653	0.6453	0.0006	0.8838	0.8847	0.8701	0.0004

The method of least squares was used to calculate the McAllister coefficients *a*, *b*, and *c* for sound speed and acoustic impedance, and standard deviations between the calculated and experimental values were determined (Tables 2 & 3). For all systems, the four-body model was found to be more accurate with sound speed and acoustic impedance mixture than the three-body model.

The equation was used to calculate the deviation in acoustic impedance (*Z*).

$$\Delta Z = Z - \sum_{i=1}^N x_i Z_i \quad (28)$$

The properties of liquids were previously examined using the van der Waal equation of state and the findings were approximated in an additive method. The linked models (RS and Glinski), which assume linearity with component mole fractions, were utilised to estimate the speed of sound in liquid mixtures and behaviour with component association. The fitted parameters were the association constant (*K_{as}*) and *u_{AB}*, where *u_{AB}* is the speed of sound of a pure hypothetical associate *AB* formed by combining the components *A* and *B*. When the fitted parameters are changed, the equilibrium concentrations of the species [*A*], [*B*], and [*AB*] change, and the speed of sound changes as well. The sum of squares for the deviation is calculated using the disparities between experimental and theoretical sound speed values.

Because the species *AB* is created by the association after mixing, it was presumed that three species (*A*, *B*, and *AB*) were present in solution rather than two (*A* and *B*). The pure associate's sound speed could be modelled as a fitting one with a value of *K_{as}*. The data for the liquid mixtures are listed in Tables 4-6. The values of such attributes in the tables vary depending on the position of the alkanol's hydroxyl group. The decrease in association power when the hydroxyl group is situated in a non primary location was the rationale for these findings. At all temperatures, when the mole percentage of alkanol increases, the density increases but the speed of sound falls. Conversely, as the mole fraction increases, the values of acoustic impedance fall until a certain limit is reached, after which they increase continually. At all temperatures, a similar trend was seen for all binary systems. For each model, the average deviation values in sound speed and acoustical impedance were computed (Table 5 & 6). The RS model, which assumes association, outperformed the Flory model, which assumed non-association. The three and four body interaction models developed by McAllister produce outstanding results. The average results, in general, follow the order; McA-3 < McA-4 < RS < Glinski < Flory. The variance in isentropic compressibility, *T*, with the mole fraction at various temperatures using different models for the examined systems is higher for the values derived by Figures 1&2.

Table 4. Average absolute percent deviations of speed of sound(*u*) from various theoretical models for binary liquid mixtures.

1-Butanol+n-Dodecane							
Average Absolute % deviation							
T/K	<i>K_{as}</i>	<i>u_{ab}</i> (m/s)	<i>u_{Flory}</i> (m/s)	<i>u_{RS}</i> (m/s)	<i>u_{Glinski}</i> (m/s)	<i>u_{McA3}</i> (m/s)	<i>u_{McA4}</i> (m/s)
288.15	0.006	1278.25	1.07	0.04	0.22	0.05	0.02
298.15	0.007	1275.25	2.07	0.14	0.36	0.04	0.02

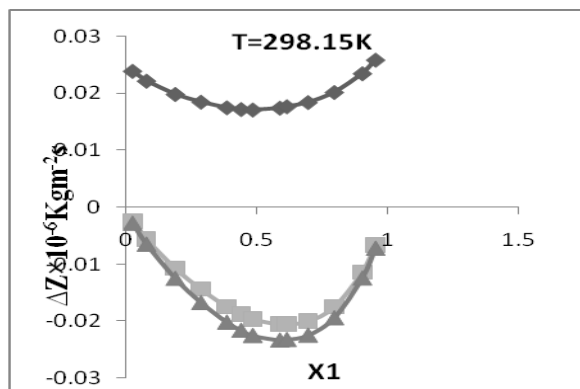
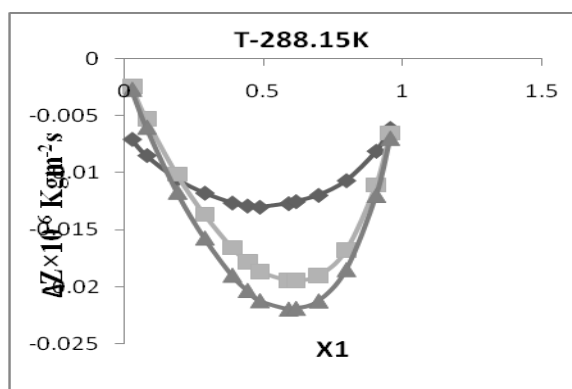
308.15	0.009	1215.25	0.29	0.23	0.52	0.04	0.02
318.15	0.04	1185.25	1.85	0.15	1.15	0.04	0.01
2-Butanol+n-Dodecane							
288.15	0.02	1250.25	1.30	0.20	0.37	0.07	0.03
298.15	0.03	1225.25	1.83	0.24	0.63	0.06	0.03
308.15	0.04	1225.25	0.40	0.26	0.90	0.05	0.03
318.15	0.03	1185.25	2.13	0.10	0.82	0.03	0.12

Table 5. Average absolute percent deviations of acoustic impedance (Z) from various theoretical models for binary liquid mixtures.

1-Butanol+n-Dodecane

Average Absolute % deviation

T/K	K_{as}	$Z_{ab} \times 10^{-6}$	Z_{Flory}	Z_{RS}	$Z_{Glinski}$	Z_{Mc3}	Z_{Mc4}
288.15	0.006	1.00	1.07	1.36	1.53	0.02	0.02
298.15	0.007	0.96	2.07	1.49	1.69	0.02	0.02
308.15	0.009	0.95	0.29	1.62	1.88	0.02	0.02
318.15	0.04	0.91	1.85	1.28	2.55	0.02	0.02
2-Butanol+n-Dodecane							
288.15	0.02	1.00	1.30	1.00	1.61	0.04	0.02
298.15	0.03	0.96	1.80	1.00	1.92	0.03	0.03
308.15	0.04	0.92	0.40	0.99	2.20	0.04	0.03
318.15	0.03	0.88	2.13	1.24	2.16	0.05	0.03



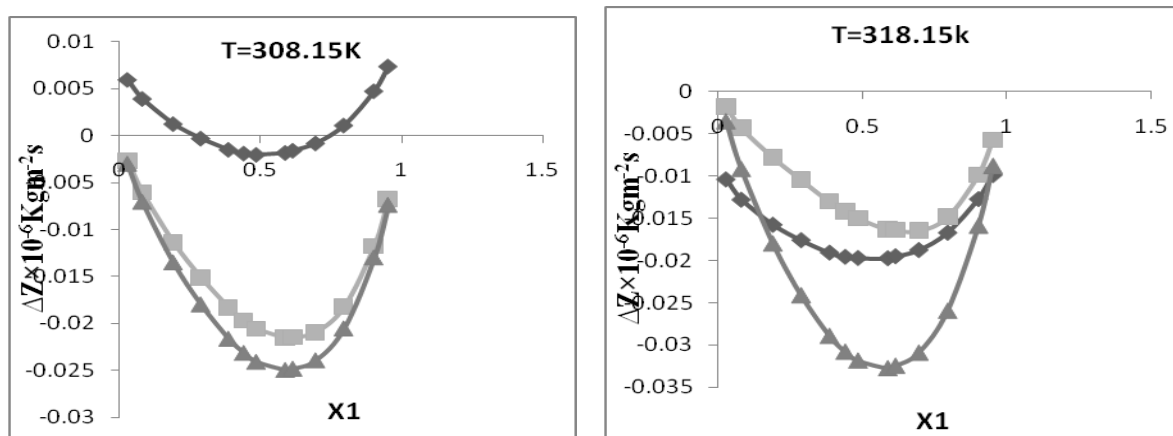


Fig.1 Deviation in the acoustic impedance (ΔZ) with the mole fraction for (x_1) 1-butanol + $(1-x_1)$ dodecane : \blacklozenge , Flory model, \blacksquare , Ramaswamy and Anbananthan model, \blacktriangle , model suggested by Glinski.

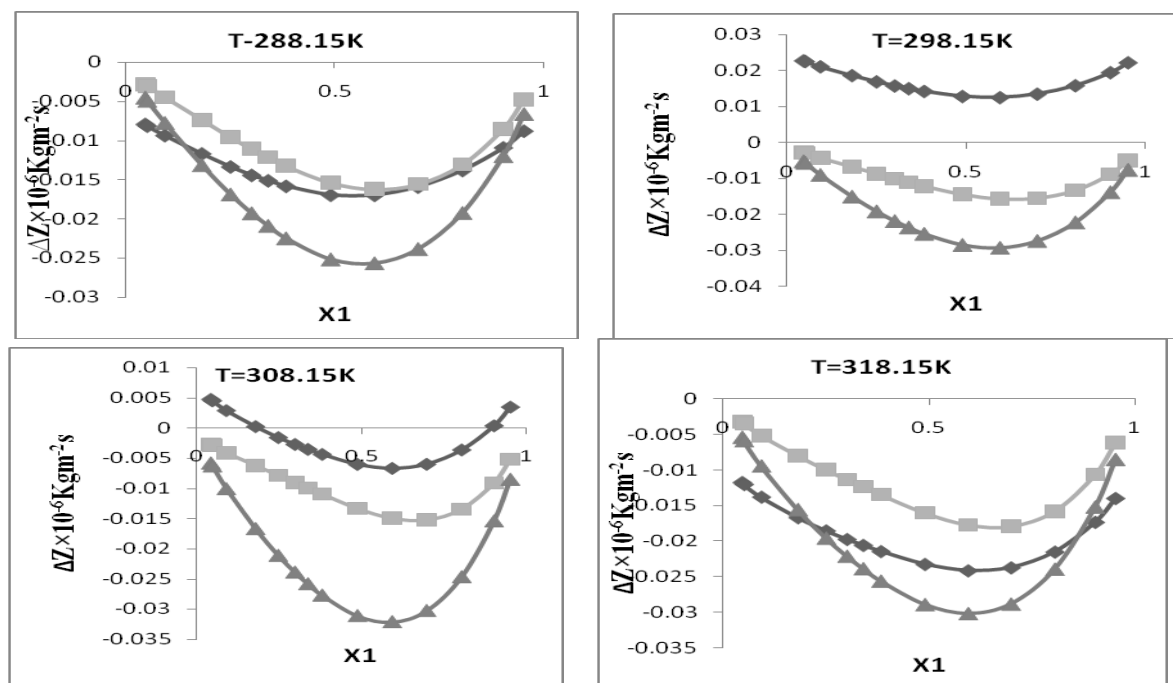


Fig. 2 Deviation in the acoustic impedance (ΔZ) with the mole fraction for (x_1) 2-butanol + $(1-x_1)$ dodecane : \blacklozenge , Flory model, \blacksquare , Ramaswamy and Anbananthan model, \blacktriangle , model suggested by Glinski.

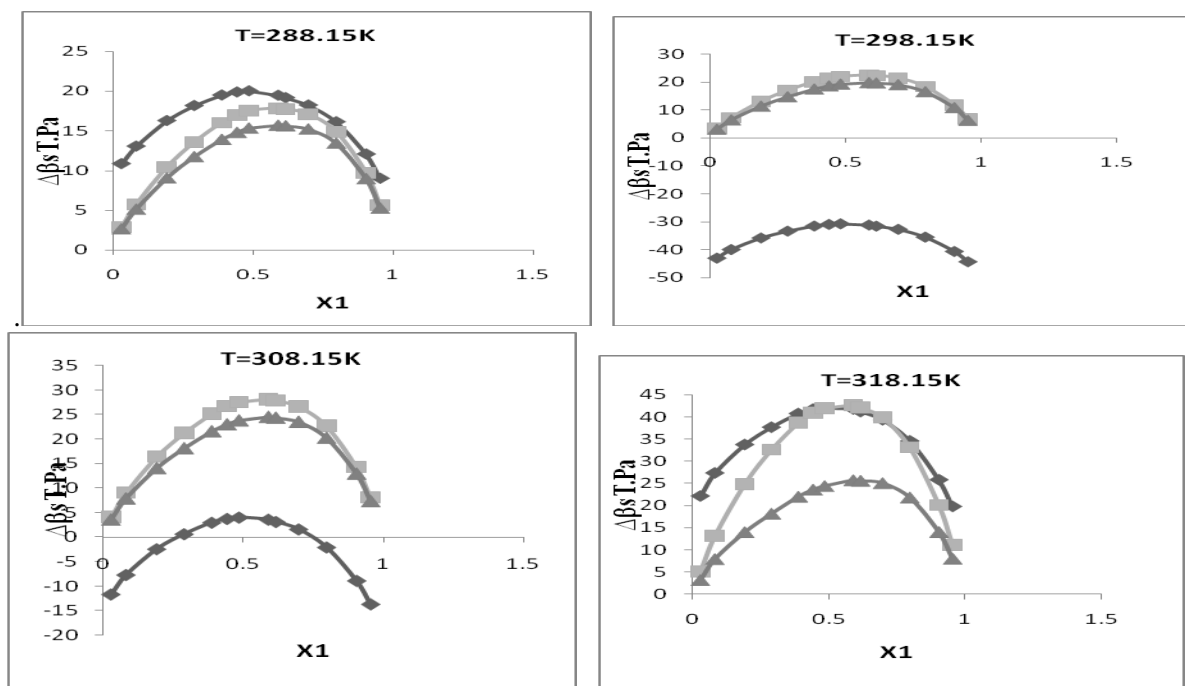
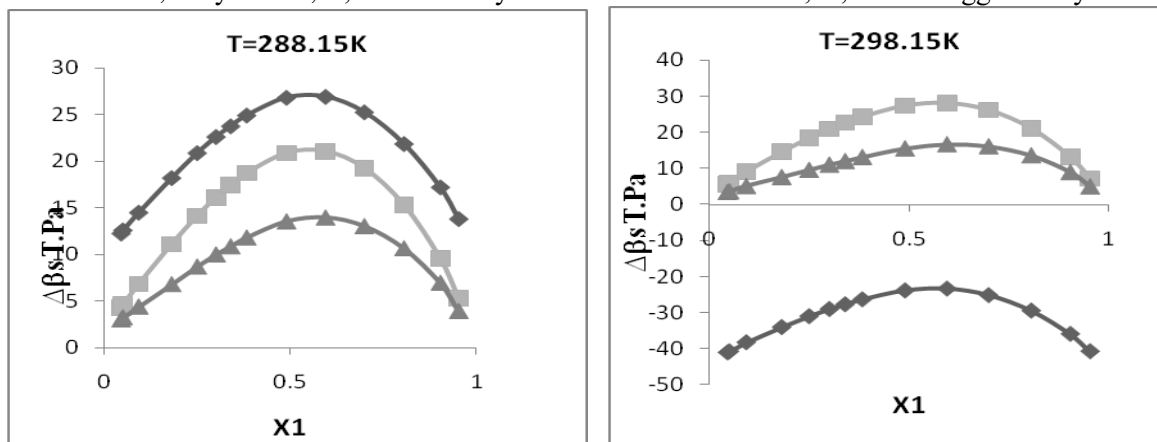


Fig. 3 Deviation in the isentropic compressibility (Δk_T) with the mole fraction for (x_1) 1-butanol + ($1-x_1$) dodecane : \blacklozenge , Flory model, \blacksquare , Ramaswamy and Anbananthan model, \blacktriangle , model suggested by Glinski .



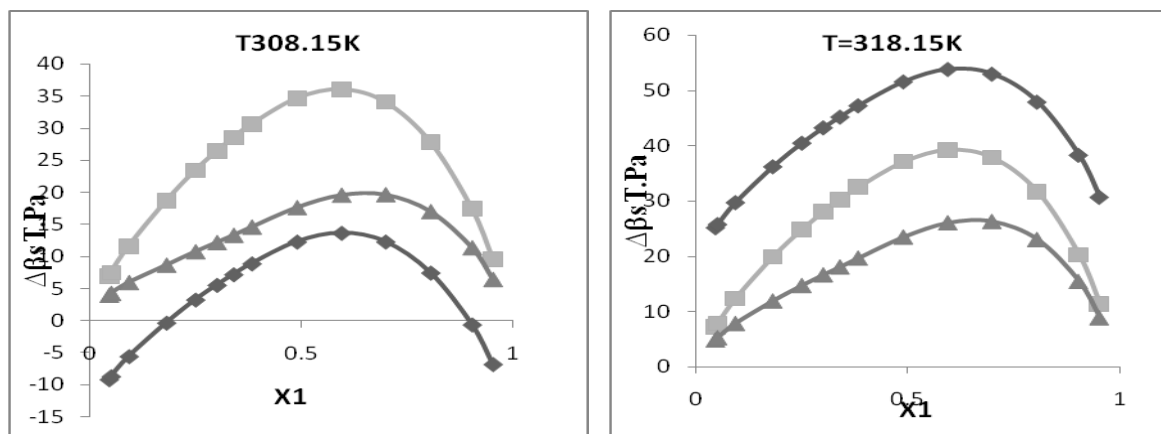


Fig. 4 Deviation in the isentropic compressibility ($\Delta\beta_{s,T}$) with the mole fraction for (x_1) 2-butanol + ($1-x_1$) dodecane : \blacklozenge , Flory model, \blacksquare , Ramaswamy and Anbananthan model, \blacktriangle , model suggested by Glinski.

As seen in alkyl chain alkanol + long chain alkane systems [1,32] they are positive across the whole composition range and grow with temperature. At all temperatures, the computed T values for the 2-butanol system are larger

than those for the 1-butanol system. The various capacities of self association of the two alkanols can easily explain the observed temperature and composition relationships. Due to its increased steric hindrance, 2-butanol has a weaker connection, which increases the breakdown of the alcohol structure by the alkane molecule, implying a higher Temperature. Different models were used to plot the variance in acoustic impedance, Z, with the mole fraction at various temperatures (Figures 3–4). The RS model demonstrated greater changes in isentropic compressibility than the Flory model for the 2-butanol system. For 1-butanol, the Glinski model performed better than the Flory model. The patterns in all of the graphs were nearly identical and showed positive changes as the temperature rose, indicating that higher temperatures result in stronger interactions between liquid molecules. Figures 3-4 indicate that all of the models' acoustic impedance deviations, ΔZ , are negative. The values of acoustic impedance deviation, ΔZ , are in this order: Flory model RS model Glinski. Negative acoustic impedance deviations in all systems are caused by a molecular association between the hydroxyl and alkane molecules, resulting in the formation of a hydrogen bond, and show weak interactions between the components due to packing effect and dipolar-dipolar interactions at all temperatures. Positive acoustic impedance variations, on the other hand, are caused by significant interactions between the component liquids in all systems. Self-

association of molecules is more important than packing effect for positive deviations. Negative deviations, on the other hand, are dominated by the packing effect and dipolar-dipolar interactions. The relative strength of these two opposing influences determines the actual sign and size of deviations.

4. CONCLUSIONS

Finally, the computed findings of sound speed, acoustic impedance, and isentropic compressibility from the RS model assuming association were shown to be superior to those obtained from the Flory model assuming non-association. The packing effect, association features, and dipolar-dipolar interactions are all explained in the McAllister three and four body interaction models, which produce good results. Except for the Flory model, acoustic impedance variances, Z, are almost negative. The least variations are found in the McAllister three and four body interactive models. Positive deviations in isentropic compressibility for all systems are caused by molecular self association and reveal substantial interactions between the components at all temperatures. Positive acoustic impedance variations, on the other hand, are caused by significant interactions between the component liquids in all systems. Self-association of molecules is more important than packing effect for positive deviations. Negative deviations, on the other hand, are dominated by the packing effect and dipolar-dipolar interactions. The relative strength of these two opposing influences determines the actual sign and size of deviations. The observed values were also utilised to evaluate a number of predictive models that are used to estimate qualities in binary mixes. All of the models were

found to describe the fluctuation of the magnitude of the attributes with the length of the alkanol chain in a qualitative fashion.

ACKNOWLEDGMENT

The authors would like to thank staff at the Department, VSSD College, Kanpur and Bhavan Mehta Mahavidyalaya, Bharwari, Kaushambi for their wishes and cooperation.

REFERENCES

1. Peleteiro J, Troncoso J, Valencia JL, Souto-Caride M, González - Salgado D. Thermodynamic Properties of Dodecane + 1-Butanol and + 2-Butanol Systems. *J. Chem. Eng. Data.* 2004; 49:1789–1793.
2. Marcel Dekker, Solvent Extraction Principles and Practice. 2nd Ed - Jan 524: ISBN 0-8247-5063-2 : Rydberg et al; 2004
3. Mellan I, Industrial Solvents; New York. Van Nostrand Reinhold: 482–88,1950 cited in Butanols: four isomers, Environmental Health Criteria monograph No. 65, Geneva: World Health Organization, ISBN 92-4-154265-9;1987.
4. Doolittle AK, The Technology of Solvents and Plasticizers. New York: Wiley: 644–45.1954, cited in Butanols: four isomers, Environmental Health Criteria monograph No. 65, Geneva: World Health Organization ; 1987: ISBN 92-4-154265-9;1987.
5. Nain AK, Densities and Volumetric Properties of Binary Mixtures of Formamide with 1-Butanol, 2- Butanol, 1,3-Butanediol and 1,4-Butanediol at Temperatures between 293.15 and 318.15 K. *J Solution Chem.* 2007; 36:497–516.
6. Bonte W. Congener Substances in German and foreign beers; *Blutalkohol* 16: 108–24,1979, cited in Butanols: four isomers, Environmental Health Criteria Monograph No. 65, Geneva: World Health Organization, ISBN 92-4-154265-9; 1987: [Online] Available: <http://www.inchem.org/documents/ehc/ehc/ehc65.htm>.
7. Monich JA, Alcohols: Their Chemistry, Properties, and Manufacture; New York: Chapman and Reinhold ; 1968, cited in Butanols: four isomers, Environmental Health Criteria monograph No. 65, Geneva: World Health Organization, ISBN 92-4-154265-9, 1987.
8. Amundsen JR, Goodwin J, Wetzel WH. Water-Soluble Pentachlorophenol and Tetra chlorophenol wood-treating systems; 1979.
9. Antoni D, Zverlov V, Schwarz WH. Biofuels from Microbes. *Applied Microbiology and Biotechnology.* 2007; 77: 23–35.
10. Shukla RK, Dixit SN, Jain Pratima, Mishra Preeti, Sharma Sweta. Ultrasonic Velocity and Isentropic Compressibility of Binary Fluid Mixtures at 298.15 K . *Orbital Elec.J. Chem.* 2010; 2: 356-364.
11. Shukla RK, Kumar Atul, Srivastava Kirti, Yadav Shilpy. A Comparative Study of PFP and BAB Models in Predicting the Excess Thermo-Acoustical and its allied properties of Liquid Ternary Mixture at 298.15 K. *J. Molliq. Liq.* 2008; 140: 25-32.
12. Shukla RK, Kumar Atul, Awasthi Naveen, Srivastava Urvashi, Srivastava Kirti. Excess Volume and Surface Tension of Some Flavoured Binary Alcohols at Temperatures 298.15, 308.15 and 318.15 K. *Phys. & Chem. Liq.* 2018; DOI: 10.1080 /003 19104.2018. 1531409.
13. Dubey Gyan. Study of Densities, Viscosities, and Speeds of Sound of Binary Liquid Mixtures of Butan-1-ol with n-Alkanes (C6, C8, and C10) at T = (298.15, 303.15, and 308.15) K. *The Journal of Chem. Thermodyn.* 2008; 40 (2): 309–320.
14. Poling BE, Prausnitz, JM, Connell O. The Properties of Gases and Liquids; Macgraw Hill: New York; 2001.
15. Shukla RK, Kumar Atul, Srivastava Kirti, Yadav Shilpy. Comparative Study of Compressibilities of Ternary Liquid Systems from two Liquid Models at 298.15 K, *Indian J. Pure & Appl.Phys.* 2007; 45: 726-732.
16. Ta, Ching. Tu, Chein-Hsiun. Densities, Viscosities, Refractive Indexes, and Surface Tensions for Binary Mixtures of 2-Propanol + Benzyl Alcohol, + 2-Phenylethanol and Benzyl Alcohol + 2-Phenylethanol at T = (298.15, 308.15, and 318.15) K. *J. Chem. Eng. Data.* 2007; 52: 1760-1767.
17. Ramaswamy K, Anbanathan D. *Acustica.*1981; 48: 281-282.
18. Gliniski, J. Determination of the Conditional Association Constants from the Sound Velocity Data in Binary Liquid Mixtures. *J. Chem. Phy.* 2003;18: 2301-2307.
19. Abe A, Flory P J. The thermodynamic properties of mixtures of small non-polar molecules. *J. Am. Chem. Soc.* 1965; 82: 1838-1845.
20. McAllister R.A. The Viscosity of Liquid Mixtures. *AIChE J.* 1960; 6: 427-431.
21. Redlich O, Kister AT. Thermodynamics of Nonelectrolytic Solutions:Algebraic Representation of Thermodynamic Properties and the Classification of Solutions. *Ind. Eng. Chem.*1948; 40: 345-348.
22. Prigogine I, Bellemans A, Mathod VA. *Molecular Theory of Solutions: North-Holland: Amsterdam; 1957.*
23. Prigogine I, Saraga L. Test of Monolayer Model for Surface Tension of Simple Liquids. *J. Chem. Phys.*1952; 49: 399-407.
24. Patterson D, Rastogi AK. The Surface Tension of Polyatomic Liquids and the Principle of Corresponding States. *J. Phy. Chem.* 1970; 74: 1067-1071.
25. Auerbach N. *Experientia.* 1948; 4: 473.
26. Pandey JD, Pant N. Surface Tension of a Ternary Polymeric Solution. *J. Am. Chem. Soc.* 1982; 104:3299.
27. Natta G, Baccaredda M. *Atti Accad. Naz. Lincei.* 1948; 4: 360.
28. Reis JCR, Santos AFS, Dias FA, Lampreia IMS. Correlated Volume Fluctuations in Binary Liquid Mixtures from Isothermal Compressions at 298.15 K *Chem. Phys. Chem.*2008; 9: 1178-1188.
29. Pfeiffer H, Heremans K. The Sound Velocity in Ideal Liquid Mixtures from Thermal Volume Fluctuations. *Chem. Phys. Chem.*2005; 6: 697-705.
30. Roseveare WE, Powell RE, Eyring H. The Structure and Dynamics of Liquids, *J. Appl. Phys.*1941; 12: 669-679.
31. Pandey JD, Verma Richa. Inversion of the Kirkwood-Buff theory of solutions. Application to binary systems. *Chem. Phys.*2001; 270: 429-438.
32. Khirwar M S,Singh A K, Singh S K,Rawat M K, Prakash Gyan.Ultrasonic Study of Calcium Soaps (Laurate and Myristate).*J Pure Appl.Ultrason.*2022;44;1-6.