Physico-Chemical Parameters and their Influence in Organic/In-organic Fluids – Mini Review

Subramanian Nithiyanantham [1,*] (ID)

[1]   Post Graduate and Research Department of Physics, Thiru.Vi. Kalyanasundaram Govt Arts and Science College, Thiruvaur, Tamilnadu, India – 610003
*   Correspondence: s_nithu59@rediffmail.com (S.N.);

Abstract: The ultrasonic velocity, density, and viscosity of organic/inorganic liquid mixtures at various temperatures. The measured parameters were used to calculate acoustic/density parameters like Thermal conductivity (Kc), Relative viscosity (η_r), Non-linear parameter (B/A), Specific heat at constant pressure (Cp), Specific heat at constant volume (C_v), Specific heat ratio (γ), Pseudo Grunisian parameter (Γ), Gibbs's free energy (ΔG), Apparent molar compressibility (ϕv), Apparent molar compressibility (ϕc), Cohesive energy density (c), Solubility parameter (δ), Free Volume (V_f), Cohesive energy (CE) and Solvation number (Sn) and some related parameters. Different acoustic magnitudes are computed because they are crucial in investigating experimental and theoretical calculations of distinct chemical interactions. With these parameters, the possible interactions among the molecules, constitutions, and favorable and non-favorable interactions are discussed.

Keywords: ultrasonics velocity; derived parameter; molecular interaction; organic/inorganic liquid mixtures.

1. Introduction

As a continuation of past work [1-5], this paper is deployed to study the physio-chemical properties of mixes such as organic/inorganic and biomolecule mixtures. To explore the influence of the glycosyl group, which is utilized in food, agriculture, and pharmaceuticals, our research team conducted a series of studies focusing on the binary ionic solution. We aim to discuss how molecular structure and composition affect isentropic compressibility and other acoustic/thermodynamic parametersto gain a better understanding of saccharides with (amylose –straight chain and amylopectin crossed chain and amylase have different molecular natures).

The authors derive numerous thermodynamic parameters from ultrasonic velocity, density, and viscosity data to explain the physicochemical behavior of the above binary mixtures. [6]. Several parameters were computed, including Thermal conductivity (Kc), Relative viscosity (η_r), Non-linear parameter (B/A), Specific heat at constant pressure (C_p), Specific heat at constant volume (C_v), Specific heat ratio (γ), Pseudo Grunisian parameter (Γ), Gibbs's free energy (ΔG), Apparent molar compressibility (ϕ_v), Apparent molar compressibility (ϕ_c), Cohesive energy density (c), Solubility parameter (δ), Free Volume (V_f), Cohesive energy (CE) and Solvation number (Sn) [6-9].

2. Sample Preparation and Experimental

The solutions were formed with Aldrich's AnalaR-grade ingredients and purified with traditional methods [10]. Any binary and ternary solution's percentage/molality/molarity in various combinations. Double-distilled deionized water was used throughout the work. The produced solutions were allowed for two hours to attain ultimate stability and the ultrasonic measurement [11].

3. Theoretical Aspects

The following relationships were used to measure and convert/compute the measured parameters: density of the solution,

$$\rho = \frac{m}{m_w} \rho_w \qquad (1)$$

$$\eta = \frac{\rho \tau}{\rho_w \tau_w} \eta_w \qquad (2)$$

where η, ρ and τ are the viscosity, density, and time of flow of solution respectively, η_w, ρ_w, and τ_w are the corresponding quantities for water.

The calculated ultrasonic velocities come from,

$$\lambda = \frac{2d}{n}, \quad U = \lambda f \qquad (3)$$

The volume filled by a substance per unit amount of substance, as well as other relationships, were used to calculate the resulting parameters,

$$V_m = \left(\frac{M}{\rho} \right) \qquad (4)$$

The degree to which a medium is easily compressed is known as its isentropic compressibility. $\beta_T = \left(\dfrac{1.71\,x10^{-3}}{T^{4/9}\,U^2\,\rho^{4/3}} \right) \quad (5)$

where T, is temperature.

The fractional increase in length in all directions is known as expansivity.

Thermal expansion coefficient $\qquad \alpha_T = (0.019\beta_T)^{1/4} \qquad (6)$

Relaxation time $\qquad t = \left(\dfrac{4\eta}{3\rho U^2} \right) \qquad (7)$

Relaxation time $\qquad \tau = 4/3\beta\eta \qquad (8)$

Relaxation strength $\qquad \alpha_r = \left(1 - \dfrac{U^2_{exp}}{U^2_{\alpha}} \right) (9)$

were, $U_{\alpha} =$ is taken us 1600 ms^{-1},

A parameter describing the flow resistance a fluid exhibits(Newtonian Fluids), relative viscosity(η_r) is the measure of the ratio of the velocity of solution (η_s) and viscosity of solvent (η_o)

Relative viscosity $\qquad \eta_r = \left(\dfrac{\eta_s}{\eta_o} \right) \qquad$ (10)

When a chemical reaction occurs in the atmosphere, the pressure is constant, hence the internal pressure is used to calculate the reaction's enthalpy. (π_i) and molar volume (V_m)

Enthalpy $\qquad H = \pi_i V_m \qquad$ (11)

Activation Energy $\qquad E_a = RT[\ln \eta V_m] \qquad$ (12)

were, R- is Universal gas constant,

Cohesion is the force of attraction between the molecules of different substances [H2O + Dextrin with Amylase], and it differs for different types of substances since surface tension (σ) is fundamentally a molecular characteristic. The force of attraction between the molecules of the same substances is known as cohesion, on the other hand.,

To estimate the surface tension depends on the density (ρ) and the velocity (η).

Surface Tension $\qquad \sigma = 6.3 \times 10^{-4} U^{3/2} \rho \qquad$ (13)

Van der walls constant $\qquad b = \dfrac{M}{\rho} - \left(\dfrac{RT}{\rho U^2} \right) \left(\left(1 + \dfrac{MU^2}{3RT} \right)^{1/2} - 1 \right)$ (14)

Molecular radius $\qquad r = \left(\dfrac{3b}{16\pi N} \right)^{1/3}$ (15)

were, N- is the Avagadro's Number,

Geometrical volume $\qquad B = \left(\dfrac{4}{3} \right) \pi r^3 N$ (16)

Molar surface area $\qquad Y = \left(36 \pi N B^2 \right)^{1/3} \qquad$ (17)

Collision factor $\qquad S = \left(\dfrac{UV}{BU_\alpha} \right) \qquad$ (18)

And

Classical absorption coefficient $\qquad \left(\dfrac{\alpha}{f^2} \right) = \left(\dfrac{8\pi^2 \eta}{3\rho U^3} \right)$ (19)

Adiabatic compressibility, $\qquad \beta = 1/U^2 \rho \qquad$ (20)

Free length, $\qquad L_f = K_T \beta^{1/2} \qquad$ (21)

Internal pressure $\qquad \pi i = bRT \qquad$ (22)

Rao's constant $\qquad R = VU^{1/3} \qquad$ (23)

Wada's constant $\qquad W = V\beta^{-1/7} \qquad$ (24)

Relative association $\qquad R_A = (\rho/\rho_o)/(U_o/U) \qquad$ (25)

Acoustic impedance $\qquad Z_a = \rho U \qquad$ (26)

Thermal conductivity $\qquad K_c = 3(\rho.N_A/M)^{3/2} K_B U \qquad$ (27)

where N_A is the Avogadro's number (6.0221×1023), k_B is the Boltzmann constant ($1.38064852 \times 10^{-23}$ m^2.kg^{-2}.K^{-1}) and M is the molar mass of solution.

Relative viscosity $\qquad \eta_r = 1 + Ac^{1/2} + Bc \qquad$ (28)

Non-linear parameter, $\qquad B/A = 2 + (0.98 \times 104)/U \qquad$ (29)

Specific heat at constant pressure,

$$C_p = 5715.36 \times 10^{-4} \, M \, U / (17.1(17.1 - \rho^{1/3}.T^{1/9})) \qquad 30)$$

Specific heat at constant volume,

$$C_v = 5715.36. \, M.u.T^{5/3} / (17.1(17.1 - \rho^{1/3}.T^{1/9})) \qquad (31)$$

Specific heat ratio	$\gamma = 17.1/ T^{4/9}\rho^{1/3}$	(32)
Pseudo Grunisian parameter	$\Gamma = \gamma - 1/\alpha T$	(33)
Gibbs's free energy,	$\Delta G = kT\ln(kT\iota/h)$	(34)
Apparent molar compressibility,	$\phi_v = (1000(\rho_0 - \rho)/c\rho\rho_0) + M/\rho$	(35)
Apparent molar compressibility,	$\phi_k = (1000(\beta_s \rho_0 - \beta_{s0}\rho)/c\rho\rho_0) + \beta_s M/\rho$	(36)
Cohesive energy density,	$C = 44.2 \, T^{4/3}\rho \, U^{3/2}$	(37)
Solubility parameter,	$\delta = T^{2/3}\rho^{1/3} U^{3/4}$	(38)
Free Volume	$V_f = (M_{eff} \, u/K\eta)^{3/2}$	(39)
Cohesive energy	$CE = V_f\pi_i$	(40)
Solvation number	$Sn = M_2/M_1[1 - ((\beta)/\beta_o)][(100-x)/x]$	(41)

Where M_1, M_2 are the molecular weight of the solvent and solute, β and β_o are the adiabatic compressibility of solution and solvent [11-15].

4. Results and Discussions

In this situation, the ultrasonic velocity is shown to be concentration-dependent in various alcohols. It is obvious from the observations that the ultrasonic velocity increases linearly with a concentration in all of the alcohols. Methanol > ethanol > 1-propanol > 1-butanol > 1-pentanol is the order of ultrasonic velocity in alcohols. However, the velocity values for ethanol and 1-Propanol are similar. This could be because the ethanol utilized in the current investigation was only 99 percent pure. As a result, the existence of impurities impacts the velocity. Overall, ultrasonic velocity rises as the CH2 group of alcohols rises [16].

Some of the estimated physicochemical parameters directly or indirectly related to ultrasonic velocity have been assessed. The fluctuation of specific acoustic impedance with concentration indicates a rising tendency based on this calculation. The measurement of opposition in acoustic flow by acoustic pressure in the solution is known as specific acoustical impedance [17]. With increasing concentration, specific acoustical impedance (Z) increases. Furthermore, when the CH2 group in alcohol grows, Z also increases, reaching a maximum in 1-pentanol and a minimum in methanol. An increase in specific acoustical impedance indicates the presence of solvent-solute interactions in solutions.

The measured values of (T) show a similar trend of decreasing values, indicating that as the percentages increase, the interaction between the mixing components will get more complex [11]. The presence of molecular contacts in other systems is suggested by a minor increase in internal pressure value with concentration [9], and isentropic compressibility is increasing (T). Solution and pure solvent viscosities are, respectively, and rel is equal to / 0. The intrinsic viscosity unit, dL/g, appears to be the inverse of the concentration unit. The relaxation time and relative viscosity rise as the proportion of solute increases. Indicators of the presence of solute-solvent and solute-solute interactions include a decrease in r and Lf [5] and a rise in Z [5] with solute concentration. The evidence on viscosity backs up this claim. As concentration rises, the value of viscosities rises, implying increased viscosity [18]. A more concentrated solution with larger molarities will have more segment-segment contact [19]. The interaction between water and dextrin molecules that causes the rise in ultrasonic velocity [5],

relaxation amplitude, and relaxation time [20] could be the cause. The increasing relaxation amplitude is consistent with structural changes caused by entropy fluctuation [21], which may be utilized to assess molecular interactions. Relaxation strength decreases at all concentrations, indicating the creation of aggregation of solvent molecules surrounding the solute, which affects the structural organization of the systems. The correlation between concentration, relaxation time, and the absorption coefficient is clear [4].

The viscous relaxation period grows dramatically with increasing concentration, and the contact between component molecules becomes greater than the attractive forces between component molecules. The presence of molecular contact is shown by the structural relaxation process, which takes 10-12 seconds. Straight-chain molecules rotate less freely than molecules with the proper configuration, which could explain this tendency. Relaxation strength varies with concentration indicates several solute-solute interactions in the solution. Other researchers' findings [22,23] corroborate these findings. The presence of interactions between the elements of the mixtures is shown by the increasing trends in molar volume (Vm), surface tension (σ), and enthalpy (H). The reawakening of the solvent-solute interaction is caused by the transition of the solute from closed to open chain formation. These conclusions are supported by the evolution of other parameters, such as the van der Walls constant (b), geometrical parameters (area, volume, and radius) increased as the solute concentration increased, as previously explained, and as anticipated, the collision factor decreased when the same conditions were present [24]. The activation energy (Ea) trends show that delaying the cooperative process or rearrangement of molecules in mixtures reduces the energy required for dissociation. Gibbs free energy was also confirmed the same (relaxation time). This indicates that if the cooperative process or rearrangement of molecules in mixtures takes less time, the energy required for dissociation is reduced [25,26].

Isentropic compressibility increases in all three systems, with acetone-toluene having the highest value compared to chlorobenzene and nitrobenzene. Because the free length and isentropic compressibility are connected, the acetone-toluene system has the least molecular interaction, indicating the presence of dispersion forces (or) London-type forces. Weak dipole-dipole interactions may also exist between acetone and nitrobenzene, as well as weak dipole-induced dipole interactions between acetone and chlorobenzene. As we know, molecules are not closer at lower concentrations, so free length increases; conversely, at greater concentrations, molecules are closer to each other, favoring segment-segment interaction, resulting in a decrease in free length, internal pressure, and isentropic compressibility.The rise in free length in acetone–toluene is larger than in other systems, as evidenced by isentropic compressibility values. It suggests that the increase in internal pressure may be causing the molecules to dissociate. The free length and isentropic compressibility between the molecules are less in the acetone – nitrobenzene system, as evidenced by the decrease in internal pressure, which favors the interaction between the molecules, resulting in a molecular association between acetone and nitrobenzene, as confirmed by the maximum value of ultrasonic velocity.

Thermodynamic values such as L_f, $ß_s$, π_i, α/f^2 decrease in the acetone-nitrobenzene system, indicating maximum molecular interaction, which could be due to dipole-dipole interaction, whereas in the acetone-chlorobenzene system, dipole–induced dipole interaction is observed, and in the acetone-toluene system, all of these values are greater, indicating the dispersion force exists between the molecules [27].

The derived values explain the experimental deviation values of acetone – toluene and acetone – chlorobenzene, which show positive and negative deviations, indicating that strong

interactions occur at lower concentrations and weak interactions occur at higher concentrations. If both positive and negative deviations are present, it could be due to physical interactions such as dispersion force caused by the breaking of cohesive forces acting on like molecules and rupture of associated structure, which dominates the interaction between like molecules and explains the experimental deviations in acetone – nitrobenzene. When comparing acetone – nitrobenzene to acetone – toluene, and acetone – chlorobenzene, it has been discovered that negative deviation occurs for excess values in nitrobenzene, which indicates that chemical forces may exist between the molecules. Compressibility can be qualitatively described as the closest approach of dissimilar molecules leading to a reduction in volume as the strength of interaction between the components increases. The theoretical ultrasonic values based on Impedance relation, Nomoto relation, Vandeal & Vangeal relation, and Jungie relation are given together with their error values for the acetone - toluene, acetone - chlorobenzene, and acetone - nitrobenzene systems. The impedance relation has a lower proportion of deviation than the Nomoto relation, Vandeal, Vangeal relation, and Junjie relation in all three systems. Overall, the complete theoretical model accurately predicts ultrasonic velocities near experimental values for all three binary mixtures presented in this study, demonstrating the validity of these theoretical models for binary mixtures [28].

The key parameters for determining the strength of intermolecular interactions are density, ultrasonic velocity, viscosity, and surface tension. Increases in these parameters with increasing concentration indicate a strong interaction between the medication and the solvent, which is observed to increase as the temperature rises. The reported values of unionized solute particles are frequently based on cohesive strength and, thus, molecular association in the solution. Surface tension, density, ultrasonic velocity, and viscosity all increase as aqueous co-solute NaCl solution concentration increases. This could be owing to the aqueous co-solute solution's connection with the medication due to the dipole interaction between the Na^+ and Cl^- ions and the polar solvent [29].

As the medication and co-solvent, NaCl, concentrations rise, the acoustic impedance (Z) also rises. However, as the temperature rises, Z decreases, possibly due to decreased interaction between the co-solute and the solvent. Adiabatic compressibility () refers to the measurement of intermolecular connection or dissociation. The adiabatic compressibility of the molecules is influenced by their structure, which also impacts their orientation around the liquid molecules. The decrease in adiabatic compressibility as the temperature rises and when the co-solute concentration increases, the drug-polar solvent interaction changes structurally, which makes the system less compressible. The presence of solvation of the solute over the breakdown of 2-TBP-aqueous solution aggregates is indicated by the fact that relative association (RA) increases with concentration. At any temperature, the values of molar compressibility (W) and Rao's Constant (R) measured in the overall system increase with increasing concentration, indicating that more components are present in the region, improving the medium's interactions in close packaging. The free volume (V_f) may be simply calculated and is crucial to understanding the many interactions in the solution. The progressive increase in free volume as the drug co-solvent NaCl mole fraction increases verifies the structural interaction between Na^+ and Cl^- ions and the solvent.

The distance between nearby molecules is measured by their free length (L_f). The mixing intermolecular free length determines the variance of ultrasonic speed in a solution. L_f decreases with the increasing concentration of an aqueous drug solution in the current study, demonstrating a significant interaction between the molecules of the drug and the solvent.

However, in the 2-TBP-co solute NaCl solution in water, the decrease in free length demonstrates the structure-enhancing behavior of the co-solute and the medication. The equation was used to compute the partial molar volume of an aqueous drug solution and 2-TBP-NaCl solutions[30, 31].

The variation of adiabatic compressibility (b) concerning the mole fraction of aniline is given from the observations. The observed data shows that the value of adiabatic compressibility decreases as the mole fraction of aniline increases, and the adiabatic compressibility value increases as the temperature rises. Ali and Nain [32] obtained similar observations in their binary mixtures, reporting that the interactions weaken as the temperature rises. The relationship between intermolecular free length (L_f) and mole fraction is shown. The value of intermolecular free length drops as the mole fraction of aniline increases, and the decrease in intermolecular free length (L_f) implies significant intermolecular interactions [33] between the liquid mixture's components. The intermolecular free length also increases as the temperature rises. The ultrasonic velocity should increase if the intermolecular free length reduces due to mixing components, according to a model presented by Eyring Kincaid [34]. The change of acoustic impedance (Z) with regard to aniline mole fraction is highlighted, and it is obvious that the value of acoustic impedance increases with aniline mole fraction. This backs up Garcia et al.[35] and Oswald et al.[36] claims of strong molecular interactions. The mole fraction increases the surface tension of the mixture. Strong interaction in a liquid mixture, according to Karla Granados [37], raises the (r) value of the mixture. This indicates that the interactions in the mixture are strong, as evidenced by the rise in (r) values as the mole fraction increases.

It also demonstrates that the decrease in surface tension as the temperature rises supports the fundamental nature of surface tension in creating interfaces with the movement of species with high surface-tension liquid and low surface-tension vapor states. Both of these metrics (L_f) are found to decrease as concentration increases. Furthermore, these values decrease when the number of people in the CH2 group grows. With concentration, the intermolecular free path length reduces, implying that the distance between the solute, lacosamide, and solvent molecules decreases. As a result, as the distance between two points reduces, velocity increases. The solution's compressibility is primarily owing to free solvent molecules around the solute, i.e., drug molecules. Compressibility reduces when there is a substantial connection between the solvent and the lacosamide molecules, which is the case in our investigation. As the concentration of lacosamide rises, molecular connections become stronger, and newly formed aggregates reduce adiabatic compressibility.

The reduction in relaxation strength (r) with concentration implies that solvent-solute interactions predominate in the examined solutions. The values further show that Rao's molar sound function (Rm), molar compressibility (W), and van der Waals constant (b) all increase as concentration increases. The variation of Rao's molar function (Rm) with concentrations is found to rise linearly for all of the examined alcohols. The least-square equation and correlation coefficient values are for some of the examined parameters. The correlation coefficient for Rao's molar sound function, van der Waals constant, and molar compressibility is almost unity. This means that while there are interactions between medication molecules and alcohol molecules, no complexes are formed. Another metric known as the solvation number confirms the type of interactions of lacosamide medication with alcohols (Sn). This provides information about a solute's ability to build or break structures in various solvents. It's possible for the solvation number to be positive or negative. The solvation number of lacosamide is positive

for all of the alcohols examined. It increases with increasing concentration for all alcohols. However, at larger concentrations, it becomes nearly constant in some circumstances. The positive solvation number implies that lacosamide tends to build structures in alcohols. This demonstrates that lacosamide and alcohol molecules have significant molecular interactions.

The thermal conductivity of a solution is also shown to decrease linearly with concentration, and this variance is attributed to numerous phenomena such as Brownian motion, clustering, and so on [38]. Thermal conductivity decreases with concentration, just as intermolecular free path length decreases. Thermal conductivity decreases as solute-solvent interaction increases with concentration, which could be related to a decrease in Brownian motion. The sequence of thermal conductivity in different alcohols is methanol > ethanol > 1-propanol > 1-butanol > 1-pentanol, i.e., it diminishes as the number of CH_2 alcohol groups increases.

5. Conclusions

The calculated acoustical parameters were calculated using the measured ultrasonic velocity, density, and viscosity values for various aqueous/non-aqueous systems, and probable interactions are described. At higher molarities, a hydrogen bond occurs between a glycosyl bond (C-O-C), and the structure of dextrin changes from a closed ring to a straight chain, according to the findings. The sign and magnitude of these quantities have been explored in terms of dipole-dipole interactions between the mixing components. Negative and positive deviations are detected in entire systems for excess values that describe the molecular interaction between the components over the complete range of mole fraction at 303 K. The experimental values for all three binary mixtures agree with the theoretical values. These findings point to the presence of substantial intermolecular interactions between the liquid mixture's components. The temperature has also been shown to reduce the strength of molecular interactions.

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