

Investigation of Excess Parameters for Aqueous Molecular Interactions 3-Pentanol in Methyl Methacrylate at Various Temperatures and 2 MHz Frequency

Kinnake S. V.¹, Gawali S. R.²

^{1,2} Dr. Ambedkar College, Chandrapur (M. S), (India)

Abstract: An The measurement was done using an ultrasonic interferometer (Model No. F-81, Mittal type). the binary liquids (ρ), (η), and (U) made up of 3- Pentanol with Methyl methacrylate. Along its whole compositions, were measured at 298K,303K and 308K. and at a frequency of 2Mhz. These data were used to calculate different acoustic characteristics viz., (β_a), (Z), (L_f), (α). The Excess Variables Viz., (β_a^E), (Z^E), (L_f^E), (V_f^E), (Π_i^E), (τ^E), (ΔG^E) have been calculated as well.

Keywords: Methyl methacrylate, Excess Parameters, 3-Pentanol, *ultrasonic* velocity.

Introduction

Understanding the intermolecular interactions between molecules, which are useful in commercial and technical processes, is greatly helped by ultrasonic examination of liquid mixtures. This topic has been investigated in relation to changes in liquid concentration for a number of binary mixes [1]. The size of the pure component of the mixtures has an impact on the strength of numerous associations, molecular mobility, and interactions, all of which have been studied using the acoustical and thermodynamic parameters.

According to these methodologies, the ultrasonic technique is more commonly used due to its affordability, simplicity, shorter time requirement, and more accurate results. This study aims to investigate the range of aqueous thermodynamic variable [2].

“To determine the nature of the molecular environment, an effort has been made to investigate the interaction between the higher alcohol, specifically 3-pentanol, and methyl methacrylate. The goal is to enhance the dispersion of drugs within polymer matrices.”

II. EXPERIMENTAL METHODS AND MATERIALS

3-Pentanol (molar mass = 88.15 gm/mol) and methyl methacrylate (molar mass = 100.12 gm/mol) were synthesized as solvents in solutions of varying concentrations (mol/kg). Using, an electronic balance equipped with a 10 mL specific gravity bottle. The densities (ρ) of these binary solutions were precisely calculated with a precision of ± 0.1 kg/m³. The solutions' viscosities (η) were measured with an accuracy of ± 0.1 Pa using Ostwald's viscometer calibrated with twice-distilled water for one second [3-4].

These essential factors distinguish various drug-based systems. Within polymers are 0, 0.1, 0.9, and 1. At temperatures of 298K, 303K, and 308K, mol/kg was found. The temperature is maintained with a precision of 0.05°C using thermostatically regulated water circulation systems [5].

The formulas given below were utilized to evaluate

$$1. \quad \text{Adiabatic Compressibility } (\beta_a) = \frac{1}{U^2 \rho} \quad \text{Kg}^{-1}\text{ms}^2 \quad (1)$$

$$2. \dots\dots\dots (L_f) = K_T \beta_a^{1/2} \quad (2)$$

Where, the Jacobson's constant,

$$K_T = (93.875 + 0.375 \times T)$$

$$3. \quad \text{Acoustic Impedance } (Z) = \rho \times U \quad \dots \quad (3)$$

The various excess values like β_a^E , L_f^E , Z^E , V_f^E , Π_i^E , τ^E and ΔG^E .

The relationship listed below was used to evaluate the examined solutions.

$$4. \quad Y^E = Y_{\text{exp}} - (x_1 y_1 + x_2 y_2) \quad (4)$$

Where, Y^E is the excess thermoacoustical parameter. Mole fraction of solute and solvent are given by x_1 and x_2 respectively. Y_{exp} is experimentally determined parameter.

III. RESULT AND DISCUSSION

Table 1-3, Provides data from experiment (ρ), viscosity (η), (U) and determined the acoustic characteristics of the aqueous 3-pentanol in methyl methacrylate solution at various evaluated concentrations at various temperatures.

The three most important parameters for determining the strength of intermolecular interactions are density, ultrasonic velocity, and viscosity.

According to table 1. below, an increase in ultrasonic speed in concentration typically indicates a decrease in the medium's compressibility. This demonstrates the strong interaction between the molecules when they are closer together. when molecules are closer together. Methyl methacrylate can function as a hydrogen bond acceptor and 3-pentanol can create hydrogen bonds in systems [6-7]. Thus, increased concentration strengthens both components' dipole-dipole or hydrogen bond interactions. Additionally, a molecular interaction is suggested by increasing the viscosity as the molar concentration rises. Density drops as molar concentration rises with temperature, indicating a loosely packed molecular structure due to hydrogen bonding geometry.

on the basis of Table 2. The mixture becomes less firmly bound and more weakly interacting, with breakdown of hydrogen bonding and dominance of weaker intermolecular forces, as indicated by increasing compressibility and free length and lowering acoustic impedance.

Furthermore, based on Table 3. The development of greater, loosely bound, dynamically altered molecular clusters with cooperative relaxation behavior is indicated by an increase in relaxation time with temperature and concentration. Internal pressure and volume expansivity changes in this system show a balance between the structure-breaking effects of methyl methacrylate and hydrogen-bond-driven association from 3-pentanol [8-9].

From fig.(a) and fig. (b), It is evident that as the concentration of 3-pentanol in methyl methacrylate excess compressibility (β_a^E), and (L_r^E) rises more positively up to 0.9 mole fraction of 3-pentanol in methyl methacrylate shows Molecules are loosely packed. Weak interactions between unlike molecules (3-pentanol and Methyl methacrylate). The liquid structure is more easily compressed and has a looser binding. Methyl methacrylate partially disrupts these strong interactions [10]. In pure 3-pentanol, hydrogen bonds may break. decreased packing efficiency and increased free volume.

Figure (c) illustrates how the excess values of acoustic impedance (Z^E) reduction negatively range from 0.1 to 0.9 mole fraction of 3-pentanol in methyl methacrylate. Acoustic impedance depends on density and sound velocity; a negative deviation indicates Weaker intermolecular interactions between unlike molecules. Looser packing and increased free volume. This means the interaction between 3-pentanol and methyl methacrylate is less cohesive than pure components [11].

In the present investigation values of (Π_i) may provide some details about the nature and force existing between molecules. Fig.(d), shows the (Π_i^E) concentration 3-pentanol in methyl methacrylate. Internal pressure reflects cohesive forces within the liquid. Negative (Π_i^E) indicates reduced cohesive energy density. all of the values can be observed to be negative. Suggests dispersion forces dominate over strong specific interactions [12]. The mixture becomes less compressible and less tightly packed.

The excess relaxation time values, which are completely negative and show a reduced resistance to molecular rearrangement, are shown in Figure 6.6(e). suggests a weaker bond between molecules. This system breaks the hydrogen bonds in 3-pentanol and reduces the formation of stable compounds with methyl methacrylate. Molecules become more mobile and less arranged. reduced relaxation time and greater dipole reorientation. Compared to an ideal mixture, the molecules in the mixture reorient more quickly [13-14].

As the concentration of 3-pentanol in methyl methacrylate rises, Figure 6.6(f) shows that the excess value of free volume (V_f^E) becomes positive. There is more free space in the mixture than would be expected from an ideal mix. The packing of molecules is efficient. Weak intermolecular interactions between dissimilar molecules are typically indicated by this. Self-association is broken. 3-pentanol creates a structure with hydrogen bonds. The polarity of methyl methacrylate is higher. The interactions become weaker or less structured when they are combined. As a result, molecules become free volume, and the structure becomes loosely packed [15].

Increasing the 3pentanol concentration in methyl methacrylate to a mole fraction of 1.0 results in negative excess values, which clearly show that the molecules that make up binary liquid mixtures interact strongly. Figures 6.6(f) and 6.6(g) demonstrate the variation of excess relaxation time (τ^E), which exhibits a similar behavior to Gibb's free energy (ΔG^E) [16].

Table 1: ultrasonic velocity (U), (ρ) and (η) with respect to concentration 3 -pentanol in Methyl methacrylate at 298K, 303K and 308K at frequency 2MHz.

Mole Fraction of 3- Pentanol in methyl methacrylate	(U) (m/s)			(ρ) (Kg/m ³)			(η) (CP)		
	298K	303K	308K	298K	303K	308K	298K	303K	308K
0	1086.66	1074.66	993.77	929	928	924	0.3546	0.3051	0.2769
0.1	1197.77	1178.22	1093.33	713.2	707.3	708.3	0.363	0.3245	0.2885
0.2	1203.98	1181.77	1125.55	694	693.7	696	0.367	0.3272	0.291
0.3	1210.2	1185.33	1157.77	674.8	680.7	683.7	0.3711	0.330	0.2936
0.4	1214.875	1199.77	1163.77	667.9	668.9	669.9	0.3941	0.3494	0.3169
0.5	1219.55	1214.22	1169.77	661	657.1	656.1	0.4172	0.3689	0.3402
0.6	1222.42	1221.77	1182.88	649.6	645.75	642.8	0.5021	0.4488	0.4124
0.7	1225.30	1229.33	1187.65	638.3	634.4	629.5	0.587	0.5288	0.4846
0.8	1238.87	1235.76	1192.43	632	627.5	624.05	0.7609	0.6946	0.6408
0.9	1252.44	1242.2	1205.32	624.6	620.6	618.6	0.9349	0.8604	0.797
1	1262.66	1256.88	1218.22	616.7	611.7	609.8	1.6293	1.4829	1.3799

Table 2. The evaluated values of (β_a), (L_f), (Z), (Π_i), Relaxation time (τ), Expansivity (α) with respect to concentration of 3-pentanol in Methyl methacrylate at 298K, 303K and 308K at frequency 2MHz.

Mole Fraction of 3- Pentanol in methyl methacrylate	$\beta_a \times 10^{-10}$ (Pa ⁻¹)			$L_f \times 10^{-10}$ (m)			$Z \times 10^6$ (Kg/m ² s)		
	298K	303K	308K	298K	303K	308K	298K	303K	308K
0	9.115	9.330	10.958	0.598	0.600	0.651	1.009	0.9972	0.9182
0.1	9.773	10.184	11.810	0.614	0.627	0.675	0.854	0.8333	0.7744
0.2	9.940	10.322	11.341	0.620	0.631	0.662	0.835	0.8197	0.7833
0.3	10.118	10.456	10.911	0.625	0.635	0.649	0.816	0.8068	0.7915
0.4	10.144	10.385	11.021	0.626	0.633	0.652	0.811	0.8025	0.7796
0.5	10.171	10.322	11.138	0.627	0.631	0.656	0.806	0.7978	0.7674
0.6	10.301	10.374	11.118	0.631	0.633	0.655	0.794	0.7889	0.7603
0.7	10.434	10.430	11.262	0.635	0.6352	0.660	0.782	0.7798	0.7476
0.8	10.309	10.435	11.269	0.631	0.6353	0.660	0.7829	0.7754	0.7441
0.9	10.206	10.442	11.127	0.628	0.6355	0.656	0.7822	0.7709	0.7456
1	10.170	10.348	11.050	0.627	0.632	0.653	0.778	0.7688	0.7428

Mole Fraction of 3- Pentanol in methyl methacrylate	Internal Pressure $\Pi_i \times 10^8(\text{Pa})$			Relaxation time $\tau \times 10^{-13} (\text{S})$			Volume Expansivity $\alpha \times 10^{-23}(\text{K}^{-1})$		
	298K	303K	308K	298K	303K	308K	298K	303K	308K
0	8.335	7.768	7.674	3.878	3.416	3.641	3.950	3.780	4.482
0.1	6.829	6.474	6.343	4.257	3.965	4.088	3.865	3.850	4.454
0.2	6.822	6.500	6.295	4.377	4.052	3.960	3.975	3.952	4.250
0.3	6.813	6.529	6.250	4.505	4.140	3.844	4.093	4.057	4.067
0.4	7.061	6.697	6.482	4.797	4.354	4.191	4.271	4.157	4.299
0.5	7.308	6.860	6.705	5.092	4.569	4.547	4.451	4.257	4.535
0.6	8.034	7.568	7.350	6.207	5.587	5.502	4.996	4.754	5.000
0.7	8.707	8.217	7.961	7.350	6.618	6.549	5.529	5.228	5.538
0.8	9.945	9.468	9.224	9.413	8.698	8.666	6.253	6.052	6.442
0.9	11.048	10.596	10.331	11.450	10.781	10.642	6.900	6.806	7.136
1	14.631	13.914	13.605	19.885	18.414	18.297	9.145	8.895	9.375

Table 3. Excess Values of (β_a^E), (L_f^E), (Z^E), (Π_i^E), (τ^E), (V_f^E), and Gibb’s Free energy (ΔG^E)

with respect to Concentration of 3-Pentanol in Methyl methacrylate at 298K, 303and 308K at Frequency 2MHz.

Mole fraction of 3-pentanol on methyl methacrylate	$\beta_a^E \times 10^{-10}$ (Pa ⁻¹) at 298K	$\beta_a^E \times 10^{-10}$ (Pa ⁻¹) at 303K	$\beta_a^E \times 10^{-10}$ (Pa ⁻¹) at 308K	$L_f^E \times 10^{-10}$ (m) At 298K	$L_f^E \times 10^{-10}$ (m) At 303K	$L_f^E \times 10^{-10}$ (m) At 308K	$Z^E \times 10^6$ (Kg/m ² s) At 298K	$Z^E \times 10^6$ (Kg/m ² s) At 303K	$Z^E \times 10^6$ (Kg/m ² s) At 308K
0	0	0	0	0	0	0	0	0	0
0.1	0.5525	0.7522	0.8428	0.0131	0.0238	0.0238	-0.1319	-0.14106	-0.12626
0.2	0.614	0.7884	0.3646	0.0162	0.0246	0.0106	-0.1278	-0.13182	-0.09982
0.3	0.6865	0.8206	-0.0746	0.0183	0.0254	-0.0026	-0.1237	-0.12188	-0.07408
0.4	0.607	0.6478	0.0262	0.0164	0.0202	0.0002	-0.1056	-0.10334	-0.06844
0.5	0.5285	0.483	0.134	0.0145	0.0150	0.004	-0.0875	-0.0852	-0.0631
0.6	0.553	0.4332	0.1048	0.0156	0.0138	0.0028	-0.0764	-0.07126	-0.05266
0.7	0.5805	0.3874	0.2396	0.0167	0.0128	0.0076	-0.0653	-0.05752	-0.04782
0.8	0.350	0.2906	0.2374	0.0098	0.0097	0.0074	-0.0413	-0.03908	-0.03378
0.9	0.1415	0.1958	0.0862	0.0039	0.0067	0.0032	-0.0189	-0.02074	-0.01474
1	0	0	0	0	0	0	0	0	0

Mole fraction of 3-pentanol on methyl methacrylate	$V_f^E \times 10^{-7}$ (m ³ mol ⁻¹) At 298K	$V_f^E \times 10^{-7}$ (m ³ mol ⁻¹) At 303K	$V_f^E \times 10^{-7}$ (m ³ mol ⁻¹) At 308K	$\Pi_i^E \times 10^8$ (Pa) At 298K	$\Pi_i^E \times 10^8$ (Pa) At 303K	$\Pi_i^E \times 10^8$ (Pa) At 308K	$\tau^E \times 10^{-13}(\text{s})$ At 298K	$\tau^E \times 10^{-13}(\text{s})$ At 303K	$\tau^E \times 10^{-13}(\text{s})$ At 308K
0	0	0	0	0	0	0	0	0	0
0.1	1.1332	0.8851	1.2015	-2.1356	-1.9086	-1.9241	-1.2217	-0.9508	-1.0186
0.2	1.4964	1.3602	1.993	-2.7722	-2.4972	-2.5652	-2.7024	-2.3636	-2.6122
0.3	1.8696	1.8353	2.7745	-3.4108	-3.0828	-3.2033	-4.1751	-3.7754	-4.1938
0.4	1.7928	1.9104	2.476	-3.7924	-3.5294	-3.5644	-5.4838	-5.0612	-5.3124
0.5	1.806	2.0555	2.3475	-4.175	-3.981	-3.9345	-6.7895	-6.346	-6.422
0.6	1.0292	1.1106	1.379	-4.0786	-3.8876	-3.8826	-7.2752	-6.8278	-6.9326

0.7	0.7224	0.7657	0.9605	-4.0352	-3.8532	-3.8647	-7.7329	-7.2966	-7.3512
0.8	0.2956	0.2308	0.312	-3.4268	-3.2168	-3.1948	-7.2706	-6.7164	-6.6998
0.9	0.2988	0.2459	0.3035	-2.9534	-2.7034	-2.6809	-6.8343	-6.1332	-6.1894
1	0	0	0	0	0	0	0	0	0

Mole fraction of 3-pentanol on methyl methacrylate	$\Delta G^E \times 10^{-20}$ (KJ/mol) At 298K	$\Delta G^E \times 10^{-20}$ (KJ/mol) At 303K	$\Delta G^E \times 10^{-20}$ (KJ/mol) At 308K
0	0	0	0
0.1	-0.00172	-0.00045	-0.00117
0.2	-0.00514	-0.0042	-0.00604
0.3	-0.00856	-0.00785	-0.01081
0.4	-0.01108	-0.0109	-0.01268
0.5	-0.0137	-0.01395	-0.01475
0.6	-0.01282	-0.0131	-0.01402
0.7	-0.01274	-0.01305	-0.01369
0.8	-0.01056	-0.0104	-0.01066
0.9	-0.00978	-0.00925	-0.00963
1	0	0	0

Graphical Representation on 3- Pentanol in Methyl methacrylate at Different Temperature and 2MHz Frequency.

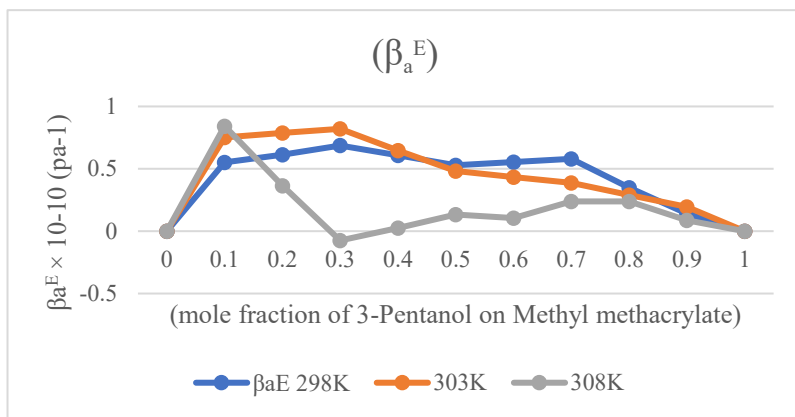


Fig.(a) Excess of Adiabatic Compressibility (β_a^E) an aqueous 3-Pentanol in Methyl Methacrylate at different Temperature.

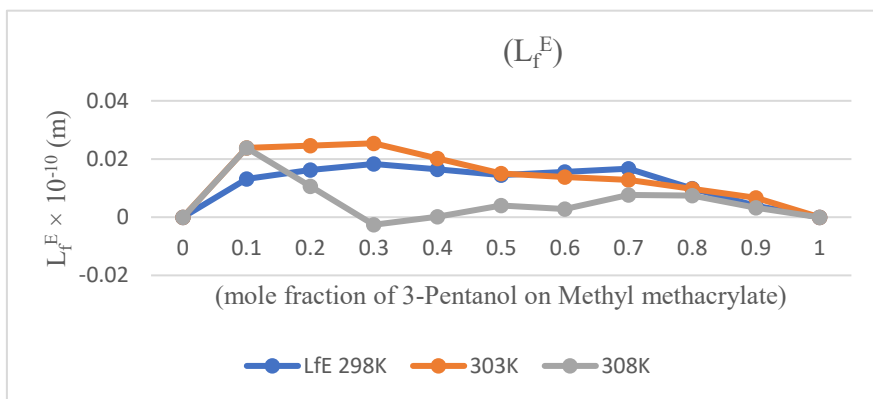


Fig.(b) Excess of Free length (L_f^E), an aqueous 3-Pentanol in Methyl Methacrylate at different Temperature.

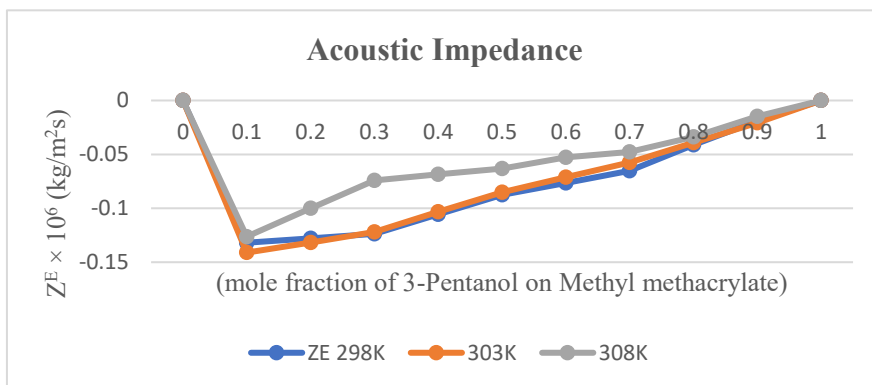


Fig.(c) Excess of Acoustic Impedance (Z^E), an aqueous 3-Pentanol in Methyl Methacrylate at different Temperature.

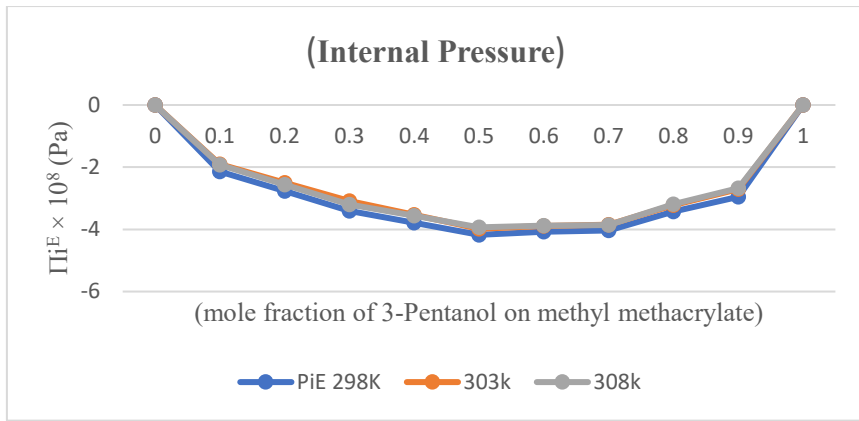


Fig.(d) Excess of Internal Pressure (Π_i^E), an aqueous 3-Pentanol in Methyl Methacrylate at different Temperature.

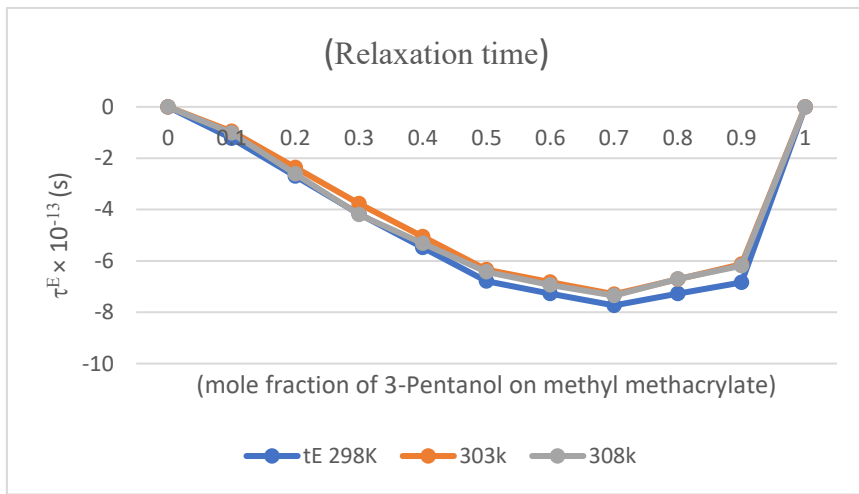


Fig.(e) Excess of Relaxation Time (τ^E), an aqueous 3-Pentanol in Methyl Methacrylate at different Temperature

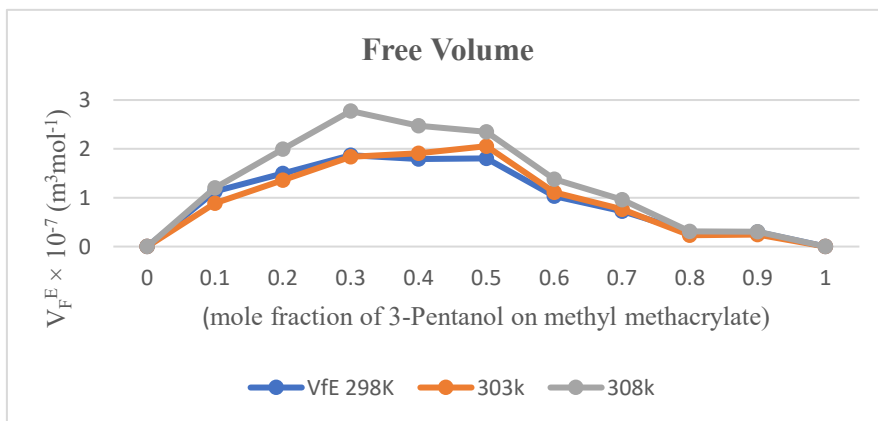


Fig.(f) Excess of Free Volume (V_f^E), an aqueous 3-Pentanol in Methyl Methacrylate at different Temperature

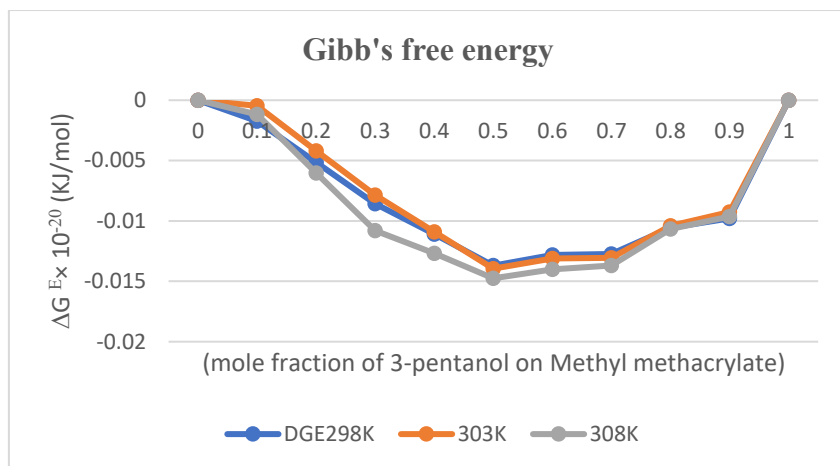


Fig.(g). Excess Gibb's Free energy (ΔG^E) of an aqueous 3-Pentanol in Methyl Methacrylate at different Temperature.

IV. CONCLUSION

The ultrasonic method is a beneficial tool for demonstrating the physical characteristics of the mixture and the presence of molecular interactions. The density, ultrasonic velocity, viscosity, and associated acoustical characteristics have been shown to be valid.

The current study applied observations of ultrasound velocity and viscosity for binary mixes of liquids of 3-pentanol with methyl methacrylate at different temperature ranges to measure the major acoustical characteristics.

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