Comparison of basic thermodynamic parameters of glyphosate with water at various frequencies

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Abstract

At different temperatures range from (303, 313, 323, 343) K for different concentrations (0.05%, 0.10%, 0.15%, 0.20%, 0.25%, 0.30%, 0.35%, & 0.40%) the basic thermodynamic properties i.e. acoustic impedance (Z), adiabatic compressibility (β), relaxation time (τ), intermolecular free length (L_f) and free volume (V_f) were calculated at 1MHz, 2MHz, 3MHz & 5MHz respectively. Solute-solvent interaction is confirmed by ultrasonic velocity and viscosity values, which increases with increase in concentration indicates stronger association between solute and solvent molecules. With rise in temperature the interaction between the solute and solvent particles decreases.

Keywords: Glyphosate, effect of temperature, effect of concentration, effect of ultrasonic frequency, acoustic impedance, adiabatic compressibility, relaxation time, intermolecular free length, free volume.

1. Introduction

Ultrasonic technique has provided an important approach to parameters for a binary or ternary solvent or pure solvent system. A significant number of studies have been carried out on this specific technique, but there is still a wide range of studies [1-7]. It teaches us about the formation of complex compounds. This is the ternary and binary mixture of glyphosate methyl ester, water and methanol. This particular mixture is used in agriculture as a pesticide. This study is interpreted in terms of molecular interactions in the chemical system. With the help of ultrasonic velocity and viscosity of the mixture, other derived parameters such as Acoustic impedance, Adiabatic compressibility, Relaxation time, Intermolecular free length and Free Volume. Glyphosate is one of the most widely used herbicides which are used in agriculture, forestry, industrial weed control, lawn, garden, and aquatic environments. Glyphosate-containing herbicides are used to control the unwanted growth of small plants known as weeds. Glyphosate can be used to ripen the green leaves along with the stem at an appropriate weather. Glyphosate also helps in increasing grain quality by reducing moistures from the crops. Glyphosate act as a plant growth regulator when applied in smaller proportion. Glyphosate also inhibits the growth of insects flying around the crop [8-13].

Measurements

To calculate velocity, ultrasonic velocity and viscosity at different concentration of dipeptides in DMSO. The basic parameters (density viscosity and ultrasonic velocity) will be calculated specific gravity bottle (10 ml) and

Oswald viscometer respectively. The other parameters as intermolecular free length, relaxation time, acoustic impedance, adiabatic compressibility and free volume will be computed by basic parameters [14-17]

Acoustics impedance:

It is the resistance which is offered to the propagation of ultrasonic wave in a material,

$$Z = \rho \times U \quad (5)$$

This impedance is used for determining the acoustic reflection and transmission at the boundary of materials having different acoustics impedances

Adiabatic compressibility:

It is defined as fractional decrease in volume per unit increase of pressure, when no heat flows out or in for temperature.

This can be determined by density of medium and speed of sound using equations of Newton's which are:

$$\beta = {}^{1}/_{[\rho(U^2)]} \quad (6)$$

Intermolecular free length:

The distances between surfaces of neighbouring molecules that is given by:

$$L_F = K_\tau (\beta)^{½} \quad (7)$$

Relaxation time:

Relaxation time for binary mixture is determined from the relation.

$$\tau = 4\,\beta\,\eta\,/3 \quad (8)$$

It can also be written as: $\tau = 4\eta/3\rho U^2$ (9)

2. Result and Discussions:

2.1. Comparison between acoustic impedance versus concentration at different frequencies by varying temperature

The acoustic impedance varies linearly with the rise in concentration indicates the absence of complex formation between Glyphosate and distilled water in solid-liquid mixture. They must exhibit opposite behaviour in liquid-liquid mixture studied due to the presence of complex formation between the molecules. At the same concentration as the temperature increases the acoustic impedance decreases[18,19]. Also with the increase in ultrasonic frequency the acoustic impedance increases as shown in table 1 to table 4.

Table 1: Experimental values of Acoustic impedance, Adiabatic compressibility, Relaxation time, Intermolecular free length and Free Volume with varying concentration & temperature at 1 MHz

Concentration (%)	Temperature (K)	Acoustic Impedance $(kg/m^2/s)(10^5)$	Adiabatic Compressibility $\beta(kg/m^2/s)(10^{-10})$	Relaxation Time τ $(sec)(10^{-10})$	Intermolecular Free length L_f $(m)(10^{-6})$	Free Volume V_f $(m^3/mole)$ (10^{-8})
0.05	303	14.217390	4.956942	5.397429	4.619820	1.997702
	313	14.151297	4.983791	4.086675	4.716031	3.053454
	323	14.076887	5.013857	3.484864	4.814203	3.908429
	333	13.994029	5.047293	2.759362	4.914477	5.596465
0.10	303	14.376316	4.875740	5.480156	4.581824	1.941891
	313	14.274089	4.922645	4.131878	4.687011	2.998070
	323	14.208547	4.949013	3.496649	4.782971	3.877779
	333	14.121620	4.986859	2.794762	4.884967	5.476984
0.15	303	14.487536	4.821589	5.543272	4.556309	1.907853
	313	14.418027	4.848399	4.150455	4.651531	2.966084
	323	14.351899	4.874325	3.510216	4.746743	3.839911
	333	14.261300	4.912525	2.811517	4.848423	5.407994
0.20	303	14.619073	4.757218	5.610117	4.525792	1.868981
	313	14.538387	4.790634	4.180672	4.623738	2.929538
	323	14.467612	4.817602	3.521384	4.719043	3.817483
	333	14.369928	4.857475	2.909537	4.821180	5.134816
0.25	303	14.717096	4.711736	5.669217	4.504106	1.841359
	313	14.652662	4.735912	4.210340	4.597254	2.896049
	323	14.577834	4.763701	3.526200	4.692569	3.807646
	333	14.495470	4.794273	2.940059	4.789713	5.043985
0.30	303	14.846430	4.656245	5.748259	4.477504	1.799245
	313	14.763232	4.686748	4.265572	4.573330	2.838506
	323	14.681359	4.716320	3.548119	4.669174	3.772952
	333	14.586010	4.750613	2.956332	4.767853	5.009489
0.35	303	14.926777	4.615229	5.828586	4.457740	1.766705
	313	14.857316	4.640172	4.320420	4.550548	2.787780
	323	14.784597	4.666381	3.558526	4.644389	3.756977
	333	14.683982	4.705189	3.027720	4.745004	4.836360
0.40	303	15.037730	4.558040	5.890409	4.430035	1.738023
	313	14.953437	4.590357	4.361507	4.526056	2.750938
	323	14.864141	4.624617	3.592600	4.623558	3.712994
	333	14.751731	4.666610	3.055273	4.725512	4.788589

Table 2: Experimental values of Acoustic impedance, Adiabatic compressibility, Relaxation time, Intermolecular free length and Free Volume with varying concentration & temperature at 2 MHz

Concentration (%)	Temperature (K)	Acoustic Impedance $(kg/m^2/s)(10^5)$	Adiabatic Compressibility $\beta(kg/m^2/s)(10^{-10})$	Relaxation Time τ $(sec)(10^{-10})$	Intermolecular Free length L_f $(m)(10^{-6})$	Free Volume V_f $(m^3/mole)$ (10^{-8})

0.05	303	14.238483	4.942266	5.381449	4.612976	2.002064
	313	14.140792	4.991198	4.092749	4.719534	3.050019
	323	14.035054	5.043790	3.505669	4.828552	3.890929
	333	13.921196	5.100244	2.788310	4.940189	5.552827
0.10	303	14.468600	4.813741	5.410472	4.552600	1.960527
	313	14.337434	4.879243	4.095448	4.666303	3.017992
	323	14.219062	4.941695	3.491479	4.779434	3.882026
	333	14.173961	4.950097	2.774160	4.866928	5.507429
0.15	303	15.225762	4.365371	5.018768	4.335395	2.055495
	313	14.555948	4.756954	4.072175	4.607456	3.008722
	323	14.415308	4.831537	3.479402	4.725863	3.865306
	333	14.324403	4.869338	2.786800	4.827064	5.443815
0.20	303	14.897326	4.581166	5.402502	4.441259	1.922566
	313	14.815510	4.613093	4.025736	4.537251	3.013629
	323	14.669288	4.686046	3.425225	4.654165	3.897582
	333	14.528292	4.752155	2.846452	4.768627	5.219841
0.25	303	15.125305	4.460842	5.367338	4.382546	1.918437
	313	15.005866	4.515590	4.014468	4.489045	3.001313
	323	14.918836	4.548421	3.366844	4.585311	3.941988
	333	14.781773	4.610354	2.827272	4.696942	5.194060
0.30	303	15.427106	4.312320	5.323673	4.308971	1.905785
	313	15.290106	4.369316	3.976666	4.415740	2.991733
	323	15.173591	4.415287	3.321650	4.517706	3.964194
	333	15.064763	4.453465	2.771415	4.616332	5.258134
0.35	303	15.738605	4.151384	5.242794	4.227801	1.912717
	313	15.590477	4.214013	3.923629	4.336553	2.996631
	323	15.461015	4.267005	3.253967	4.441197	4.017730
	333	15.335417	4.313934	2.775954	4.543440	5.161665
0.40	303	16.035906	4.008258	5.179919	4.154281	1.913841
	313	15.925842	4.046911	3.845154	4.249703	3.023559
	323	15.724584	4.132350	3.210185	4.370559	4.039957
	333	15.564145	4.192151	2.744641	4.478850	5.189484

Table 3: Experimental values of Acoustic impedance, Adiabatic compressibility, Relaxation time, Intermolecular free length and Free Volume with varying concentration & temperature at 3 MHz

Concentration (%)	Temperature (K)	Acoustic Impedance $(kg/m^2/s)(10^5)$	Adiabatic Compressibility $\beta(kg/m^2/s)(10^{-10})$	Relaxation Time τ $(sec)(10^{-10})$	Intermolecular Free length L_f $(m)(10^{-6})$	Free Volume V_f $(m^3/mole)$ (10^{-8})
0.05	303	14.270125	4.92037	5.35761	4.60275	2.00882
	313	14.151297	4.98379	4.08667	4.71603	3.05341
	323	13.993220	5.07399	3.52666	4.84299	3.87360
	333	13.858769	5.14630	2.81349	4.96244	5.51543
0.10	303	14.701966	4.66214	5.24007	4.48034	2.00816
	313	14.569706	4.72491	3.96591	4.59191	3.09161

	323	14.450439	4.78471	3.38057	4.70291	3.97711
	333	14.289112	4.87064	2.72963	4.82771	5.57464
0.15	303	15.116039	4.42897	5.09189	4.36686	2.03326
	313	14.990928	4.48490	3.83928	4.47377	3.14456
	323	14.838046	4.56016	3.28397	4.59122	4.03659
	333	14.671469	4.64169	2.65651	4.71288	5.64292
0.20	303	15.443133	4.26306	5.02737	4.28429	2.02915
	313	15.316467	4.31627	3.76670	4.38885	3.16782
	323	15.157556	4.38901	3.20811	4.50424	4.09371
	333	15.013978	4.44967	2.66527	4.61437	5.48384
0.25	303	15.952470	4.01023	4.82516	4.15530	2.07800
	313	15.830013	4.05765	3.60734	4.25534	3.25191
	323	15.664777	4.12555	3.05383	4.36696	4.24134
	333	15.428568	4.23191	2.59519	4.50004	5.53866
0.30	303	16.431814	3.80110	4.69255	4.04550	2.09498
	313	16.257834	3.86464	3.51734	4.15290	3.28025
	323	16.083149	3.93001	2.95657	4.26221	4.32595
	333	15.926517	3.98457	2.47962	4.36655	5.71566
0.35	303	16.853512	3.62030	4.57209	3.94812	2.11957
	313	16.722567	3.66276	3.41036	4.04298	3.32884
	323	16.556170	3.72117	2.83772	4.14742	4.45205
	333	16.339268	3.80014	2.44533	4.26430	5.67669
0.40	303	17.283625	3.45043	4.45903	3.85438	2.14153
	313	17.114337	3.50436	3.32965	3.95458	3.36826
	323	16.939959	3.56066	2.76607	4.05699	4.51729
	333	16.740007	3.62390	2.37260	4.16424	5.78858

Table 4: Experimental values of Acoustic impedance, Adiabatic compressibility, Relaxation time, Intermolecular free length and Free Volume with varying concentration & temperature at 5 MHz

Concentration (%)	Temperature (K)	Acoustic Impedance $(kg/m^2/s)(10^5)$	Adiabatic Compressibility $\beta(kg/m^2/s)(10^{-10})$	Relaxation Time τ (sec)(10^{-10})	Intermolecular Free length L_f (m)(10^{-6})	Free Volume V_f $(m^3/mole)$ (10^{-8})
0.05	303	14.765835	4.595551	5.003923	4.448226	2.114335
	313	14.603044	4.680211	3.837742	4.570139	3.200813
	323	14.380178	4.804593	3.339417	4.712667	4.035388
	333	14.098073	4.973070	2.718784	4.878208	5.658924
0.10	303	15.380844	4.259665	4.787710	4.282583	2.148929
	313	15.203170	4.339373	3.642302	4.400583	3.295412
	323	14.934223	4.479738	3.165090	4.550559	4.178551
	333	14.707840	4.597253	2.576417	4.690263	5.821424
0.15	303	15.925636	3.990117	4.587347	4.144870	2.198812
	313	15.754797	4.060545	3.476016	4.256855	3.387976
	323	15.535560	4.159866	2.995703	4.385086	4.324598
	333	15.302502	4.266759	2.441935	4.518530	6.010830

0.20	303	16.481236	3.742942	4.413997	4.014437	2.237215
	313	16.254428	3.832499	3.344530	4.135593	3.463212
	323	16.081021	3.899396	2.850230	4.245581	4.473427
	333	15.890321	3.972413	2.379401	4.359887	5.970924
0.25	303	16.972999	3.542484	4.262360	3.905459	2.280509
	313	16.804002	3.600901	3.201288	4.008689	3.556616
	323	16.570565	3.686853	2.729092	4.128254	4.614369
	333	16.382955	3.753210	2.301634	4.237888	6.060459
0.30	303	17.717406	3.269487	4.036269	3.751957	2.345614
	313	17.472871	3.345846	3.045170	3.864112	3.654798
	323	17.228124	3.424993	2.576645	3.978949	4.796053
	333	16.915941	3.532078	2.198031	4.111149	6.256430
0.35	303	18.239028	3.091164	3.903839	3.648204	2.386160
	313	18.059508	3.140530	2.924118	3.743675	3.735928
	323	17.823115	3.210938	2.448623	3.852604	4.972713
	333	17.567383	3.287385	2.115384	3.966189	6.328638
0.40	303	18.715788	2.942567	3.802715	3.559437	2.413150
	313	18.529728	2.989444	2.840406	3.652514	3.794544
	323	18.338177	3.038387	2.360349	3.747658	5.087984
	333	18.065525	3.111618	2.037205	3.858702	6.489506

2.2. Comparison between adiabatic compressibility versus concentration at different frequency by varying temperature

The adiabatic compressibility decreases with increase in the concentration of Glyphosate in distilled water [20]. As a result of strong intermolecular interactions between solute and solvent molecules in the binary mixture adiabatic compressibility decreases that indicates enhancement in bond strength[21]. But as the temperature increases the bond strength decreases between Glyphosate and distilled water[22]. As a result with increase in temperature the adiabatic compressibility increases as shown in table 1 to table 4. The adiabatic compressibility is higher at 333 K temperature due to decrease in bond strength and vice-versa. Adiabatic compressibility is inversely proportional to the ultrasonic frequency[23-25].

2.3. Comparison between relaxation time versus concentration at different frequency by varying temperature

The relaxation time provides information about an orientation of the molecules in space. With an increase in concentrations, the structure of the solution changes forming dissociation of molecules of mixture. Therefore viscous drag between solute and solvent molecules decreases thereby the time taken for the flow of ultrasonic waves in the viscous medium decreases. As the temperature increases, the relaxation time further decreases[26] as shown in table 1 to table 4. As it is clear from the above graphs that relaxation time is inversely proportional to the ultrasonic frequency (2MHz to 5MHz).

2.4. Comparison between intermolecular free length versus concentration at different frequency by varying temperature

The intermolecular free length decreases with increase in concentration. As the number of molecules in the give solution increases with increase in the number of solutes in it, thereby the average distance between the molecules decreases that indicates the fall in intermolecular free length with the rise in concentration. But as the temperature increases the molecules gain energy and their intermolecular free length tend to increase. Hence an Intermolecular free length is highest at 333 K temperature and vice versa[27]. The Intermolecular free length is inversely proportional to ultrasonic frequency.

2.5. Comparison between free volume versus concentration at different frequency by varying temperature

At 1MHz and 2MHz free volume slightly decreases with increase in concentration but well noticeable only at higher temperature 333 K and at 3MHz & 5MHz the free volume increases with increase in concentration and temperature. As the number of molecules increases they occupy a less volume. Also as the temperature increases volume occupied by them will further increase due to rise in movement of the molecules of the solution. Due to increase in temperature the bond between the molecules breaks and hence at highest temperature the free volume available will be more. The free volume is inversely proportional to ultrasonic frequency[28, 29].

3. Conclusion

The acoustic impedance of the glyphosate-water directly depends on concentration but inversely depends on temperature. The linear variation of acoustic impedance against the concentration as well as temperature indicates the strong interaction between glyphosate-water molecules. It is a significant factor affecting reflection and transmission of sound waves in the medium and solvent molecules. Hence it increases with increase in ultrasonic frequency. The derived parameters such as adiabatic compressibility and Intermolecular Free length shows opposite behaviour with ultrasonic velocity. They decreases with increase in concentration of the solute but exhibhits opposite trends with rise in temperature. Due to increase in the temperature the thermal energy of the system increases that cause volume expansion which increases adiabatic compressibility and Intermolecular Free length. It indicates that molecules of glyphoste-water are forming more tightly bound system. They decreases with increase in ultrasonic frequency showing stronger bond association between glyphosate-water.

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