

INTERMOLECULAR INTERACTION OF TRIPLE SUPER PHOSPHATE FERTILIZER IN AQUEOUS SOIL SALT SOLUTIONS : AN ULTRASONIC STUDY

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ABSTRACT

The ultrasonic parameters and characterization helps to forecast and understand the behavior of intermolecular interaction, strength as well as the ilk of the liquid mixture present in the system. In view of above facts, the ultrasonic velocity (U) and density (?) measurements studies on fertilizer name as Triple Super Phosphate having number of concentrations varying from 0.002-0.02 mol·kg⁻¹ in 0.2 mol kg⁻¹ aqueous soil salt solution at 293.15K temperature were undertaken during the month of March 2021 at physical science laboratory, Sardar Patel Mahavidyalaya, Chandrapur, Maharashtra. The various thermo-acoustical parameters were calculated: Adiabatic Compressibility (β), Acoustic Impedance (Z), Intermolecular Free Length (L_f), Specific Heat Ratio (γ), Non-Linear Parameter (B/A), Isothermal Compressibility (k_T), Pseudo-Grüneisen Parameter (Γ) and Internal Pressure (π_i). In the light of all the observations and discussions, it may be interpreted that: the concentration, nature of solute, nature of solvent and its position plays an important role in determining the interactions occurring in the solution. From the acoustical and volumetric parameters it is concluded that H-bonding interaction was strong at higher concentration. The thermo-acoustic and volumetric parameters exhibited the strength of molecular interaction. It is observed that the order of interaction was : Na₂SO₄>NaCl>H₂O

This kind of information can be useful in the manufacturing of more effective fertilizer by increasing their activity according to soil salinity treatment and in other application by changing the ilk of its molecule. Hence the study expose the structural sense of the experimental liquid mixture and results have been described in the light of intermolecular interaction exist in between the fertilizer-water-saline salt solutions.

(Keywords : Fertilizer, pseudo-grüneisen parameter, internal pressure, triple super phosphate, intermolecular interaction)

INTRODUCTION

Nowadays, ultrasonic field have bearded the status of an important inquest to study the properties of science, industries, metallurgy, medicine and also in agriculture (Mishra *et al.*, 2020). The ultrasonic velocity has been measured in order to understand the ilk of molecular interactions in pure, binary and ternary mixtures (Praharaj *et al.*, 2012). Acoustical parameters were calculated from the experimentally determine values of speed of sound and density of the experimental liquid mixture. Such studies as a function of concentration and temperature are useful in gaining insight into the structure and bonding between the associated molecules.

Knowledge of thermo-acoustic properties is of great importance in studying and understanding the various physico-chemical behavior and molecular interactions between various essential molecules in a living organism as well as in plants. Although, chemical fertilizers are playing a

crucial role to feed crops with nutrients they need to grow and be harvested for nutritious food posing a greater thread to sustainable agriculture (Fayera *et al.*, 2021). During the last two decades the ultrasonic study has been carried out to investigate hydration of fertilizers (Khatun *et al.*, 2018).

Fertilizers are the main constituents of Nitrogen, Potassium and Phosphorous nutrients and are quite useful for understanding the thermodynamic and physico-chemical behavior of nutrients in solution. (Rathika *et al.*, 2014). As triple super phosphate fertilizer is highly concentrated phosphorous fertilizer having 46% of di-phosphorous pentoxide (P₂O₅). It accelerate the growth of the root of the young plants and increases the resistance of the plants to freezing and drought. Thus, we report in this manuscript, the effect of TSP fertilizer on saline salt solution, which offers a way to counteract the salinity problem in agriculture.

MATERIALS AND METHODS

The liquid mixture of various weight fraction (*viz.*, 0.002-0.02 mol.kg⁻¹) of triple super phosphate in water and

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in 0.2 mol.kg⁻¹ aqueous solution of sodium chloride and sodium sulfate were prepared by taking AR grade chemicals of 99.8% purity. The ultrasonic velocity measurement carried out at a constant 293.15K temperature with the help of thermostatic water bath having an accuracy ± 1 K at a fixed 2MHz frequency digital ultrasonic velocity interferometer with an overall accuracy 0.0001 ms⁻¹.

The densities of the solutions were determined accurately using 10 ml specific gravity density bottle having accuracy $\pm 2 \times 10^{-2}$ kg.m⁻³. All the weighings were done with the help of digital electronic balance having accuracy 0.0001g.

Defining relations

For the derivation of several acoustical and thermodynamical parameters the following defining relations reported in the literature are used:

- ❖ Adiabatic Compressibility ($\hat{\alpha}$) = $1/(U^2 \hat{n})$
- ❖ Acoustic Impedance (Z) = $U \hat{n}$
- ❖ Intermolecular Free Length (L_f) = $K(\hat{\alpha})^{1/2}$
- ❖ Specific Heat Ratio ($\hat{\alpha}$) = $\left\{ \frac{17.1}{T^{4/3} \rho^{1/3}} \right\}$
- ❖ Non-Linearity Parameter (B/A) = $\left\{ 2 + \left[\frac{0.98 \times 10^4}{U} \right] \right\}$
- ❖ Isothermal Compressibility (k_T) = $\left\{ 1.33 \times 10^{-8} / (6.4 \times 10^{-4} U^{3/2} \hat{n})^{3/2} \right\}$
- ❖ Pseudo-Grüneisen Parameter (r) = $\left\{ \frac{\gamma - 1}{\alpha \times T} \right\}$
- ❖ Internal Pressure (δ_i) = $\left\{ \frac{T \times \alpha}{k_T} \right\}$

RESULTS AND DISCUSSION

The ultrasonic velocity and density of fertilizer: triple super phosphate of varying concentration in water and 0.2 mol.kg⁻¹ aqueous solution of sodium chloride and sodium sulfate increased with the increase in concentration, shown in Fig. 1 and Fig. 2 respectively. The increase in sound speed and density is accredited to the cohesion brought about by the ionic hydration and the construction of hydrogen bond between the fertilizer-water-saline salt. The fertilizer molecule form more compact structure with soil salt molecules which clearly showed the strong intermolecular interaction between the fertilizer and saline salts molecules due to the increase in the cohesive force. This functions as a material medium for sound waves. The similar results was obtained by Kumar (2012), who reported the ultrasound velocity increased with the increasing concentration of electrolyte at all temperatures.

It is observed from Fig. 3 that the adiabatic compressibility for both the salt solutions showed decreasing order with the increase in weight fraction of fertilizer in the salts solutions. This decreased in adiabatic compressibility indicating strong intermolecular interactions between the fertilizer and saline salts as compared to saline

salts and water. The similar trends occurred by the Thirumaran *et al.* (2011). They revealed that the decreased intermolecular free length after mixing the components, confirms the association of molecules.

Acoustic impedance has a direct relation with elastic property of the solution. Fig. 4, represents the behavior of triple super phosphate fertilizer in aqueous saline salt solutions at 293.15K temperature at a frequency of 2MHz. The acoustic impedance versus weight fraction of TSP fertilizer graph showed the increasing trend for both the salt solutions and confirms the molecular interaction present in the solution. Tadalkar *et al.* (2011) also observed that the acoustic impedance increased with the increase in concentration and confirms the molecular interaction between fructose with magnesium chloride was stronger than sodium chloride solutions. It is observed that the order of acoustic impedance for current work was : $\text{Na}_2\text{SO}_4 > \text{NaCl} > \text{H}_2\text{O}$.

Intermolecular free length is the distance between the surfaces of two neighboring molecules. Thus, it specifies the interaction plays between the constituent molecules. The regular decrease in the value of intermolecular free length with the increase in weight fraction of TSP fertilizer are tabulated in Table 1 and represented graphically in Fig.5. The graph clearly showed the strong packing between the components of fertilizer with saline salt solutions. Mishra and Manik (2015) found the similar behavior of experimental liquid in their work, as the concentration of solute i.e. 2-Phenylaniline in Toluene solvent increased, the values of free length exhibit decreasing trend. The observed order of variation of intermolecular free length (Lf) in water as well as in salt solution is: $\text{Na}_2\text{SO}_4 < \text{NaCl} < \text{H}_2\text{O}$

The non-linearity parameter plays a significant role in acoustic, from underwater acoustic to medicine and fertilizer. From the Table 2 it is observed that the value of non-linearity parameter showed a decreasing order while increasing the concentration of solute in both the solvents and confirms the increasing trend of internal pressure as shown in Fig. 10.

The overall trend in the isothermal compressibility (k_T) shown in Fig. 8 has been found decreased with the increase in weight fraction of fertilizer: TSP in both the saline salt solutions. The decrease in k_T values supports to the effective TSP fertilizer interaction with saline salts solutions. The decrease in k_T values with continuous increase in fertilizer concentration in weight fraction seems to be the result of corresponding decrease in free volume and hence confirms the decrease of free length. Similar results were obtained by the Basharat (2012) in his work. He found that the ternary systems (amino acid + salt + water) in aqueous 0.5m K_2SO_4 solution decreased with the addition of solute. The resultant order of isothermal compressibility is: $\text{Na}_2\text{SO}_4 < \text{NaCl} < \text{H}_2\text{O}$

The Pseudo-Grüneisen parameter (r) measures the degree of molecular or ionic association. The calculated values of r have been listed in Table 2 and a graph is plotted

Table 1. The values of Ultrasonic Velocity, Density, Adiabatic Compressibility, Acoustic Impedance and Intermolecular Free Length as a function of concentration of System (Triple Super Phosphate + 0.2M aq. Solution of (NaCl/Na₂SO₄) at temperature 293.15K

Conc. (mol·kg ⁻¹)	T=293.15K									
	U (m/s)		(Kg/m ³)		$\hat{a} \cdot 10^{-10}(\text{m}^2\text{N}^{-1})$		Z (kgm ² s ⁻¹)		$L_f \cdot 10^{-11}$ (m)	
	NaCl	Na ₂ SO ₄	NaCl	Na ₂ SO ₄	NaCl	Na ₂ SO ₄	NaCl	Na ₂ SO ₄	NaCl	Na ₂ SO ₄
0.00	1481.496	1481.496	998.200	998.200	4.56	4.56	1478829	1478829	4.36	4.36
0.2M	1494.976	1512.712	1006.435	1026.985	4.45	4.26	1504596	1553533	4.30	4.21
0.002	1497.247	1515.616	1010.186	1024.810	4.42	4.25	1512498	1553219	4.29	4.20
0.004	1498.385	1516.781	1010.591	1025.800	4.41	4.24	1514253	1555914	4.28	4.20
0.006	1499.525	1517.948	1011.448	1026.761	4.40	4.23	1516692	1558568	4.28	4.19
0.008	1500.666	1518.525	1012.068	1027.713	4.39	4.22	1518776	1560603	4.27	4.19
0.010	1501.810	1519.701	1012.696	1028.635	4.38	4.21	1520877	1563210	4.27	4.19
0.012	1502.955	1520.286	1013.301	1029.550	4.37	4.20	1522946	1565210	4.26	4.18
0.014	1504.101	1521.458	1014.100	1030.447	4.36	4.19	1525309	1567771	4.26	4.18
0.016	1505.250	1522.632	1014.532	1031.341	4.35	4.18	1527124	1570351	4.25	4.17
0.018	1506.401	1524.396	1015.412	1032.235	4.34	4.17	1529618	1573527	4.25	4.17
0.020	1507.553	1525.585	1016.368	1033.118	4.33	4.16	1532229	1576097	4.24	4.16

Table 2. The values of Specific Heat Ratio, Non-Linear Parameter, Isothermal Compressibility, Pseudo-Gruneisen Parameter and Internal Pressure as a function of concentration of System (Triple Super Phosphate + 0.2M aq. Solution of (NaCl/ Na₂SO₄) at temperature 293.15K

Conc.(mol·kg ⁻¹)	T=293.15K									
	$\gamma (\text{K}^{4/9})^{-1}(\text{kg}^{1/3}\text{m}^{-1})^{-1}$		(B/A) (m ¹ s)		$kT \cdot 10^{-11} (\text{m}^2\text{N}^{-1})$		γ		$\pi_i \cdot 10^9$	
	NaCl	Na ₂ SO ₄	NaCl	Na ₂ SO ₄	NaCl	Na ₂ SO ₄	NaCl	Na ₂ SO ₄	NaCl	Na ₂ SO ₄
0.00	0.137016	0.137016	8.61493517	8.614935	6.05	6.05	-3.12742	-3.12742	5.06	5.06
0.2M	0.136642	0.135724	8.55528918	8.478431	5.85	5.53	-3.14486	-3.17075	5.21	5.47
0.002	0.136472	0.135820	8.54534623	8.466018	5.8	5.52	-3.14854	-3.17325	5.25	5.47
0.004	0.136454	0.135776	8.54037514	8.461051	5.79	5.51	-3.14992	-3.17483	5.26	5.49
0.006	0.136416	0.135734	8.53540288	8.456084	5.77	5.49	-3.15144	-3.1764	5.27	5.50
0.008	0.136388	0.135692	8.53043382	8.453633	5.76	5.48	-3.15289	-3.17733	5.28	5.51
0.010	0.136359	0.135652	8.52545928	8.448637	5.74	5.46	-3.15434	-3.17890	5.29	5.53
0.012	0.136332	0.135611	8.52048797	8.446156	5.73	5.45	-3.15578	-3.17982	5.30	5.54
0.014	0.136297	0.135572	8.51551990	8.441190	5.71	5.43	-3.15729	-3.18138	5.32	5.55
0.016	0.136277	0.135533	8.51054642	8.436224	5.70	5.42	-3.15868	-3.18294	5.33	5.56
0.018	0.136238	0.135494	8.50557189	8.428776	5.68	5.39	-3.23322	-3.18514	5.34	5.58
0.020	0.136195	0.135455	8.50060064	8.423765	5.66	5.38	-3.16178	-3.18671	5.36	5.60

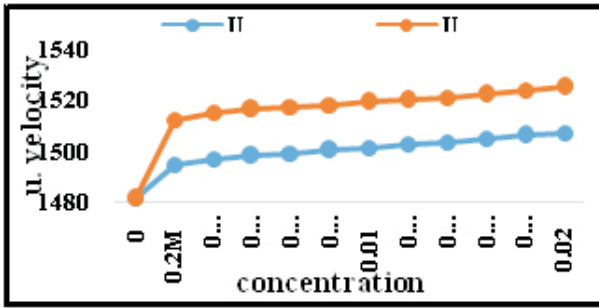


Fig. 1. Ultrasonic velocity versus concentration at 293.15K temperature.

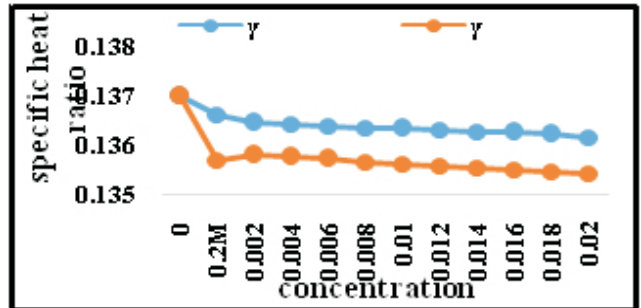


Fig. 6. Specific Heat Ratio versus concentration at 293.15K temperature.

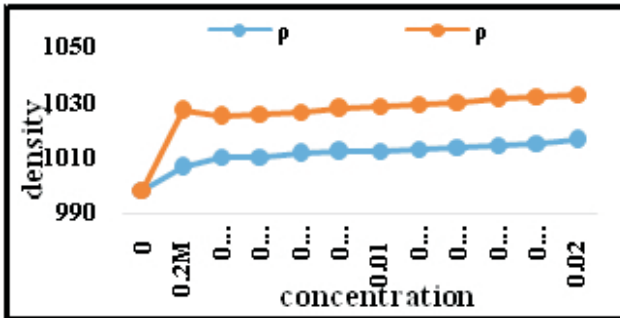


Fig. 2. Density versus concentration at 293.15K temperature.

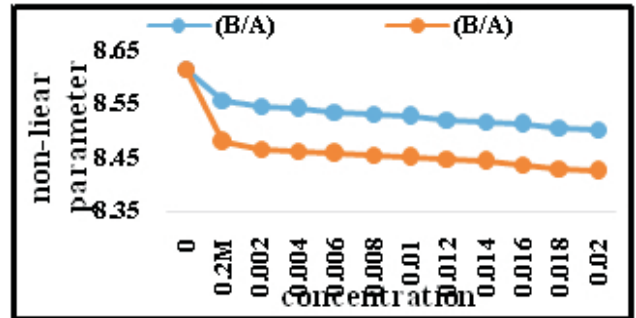


Fig. 7. Non-Linear Parameter versus concentration at 293.15K temperature.

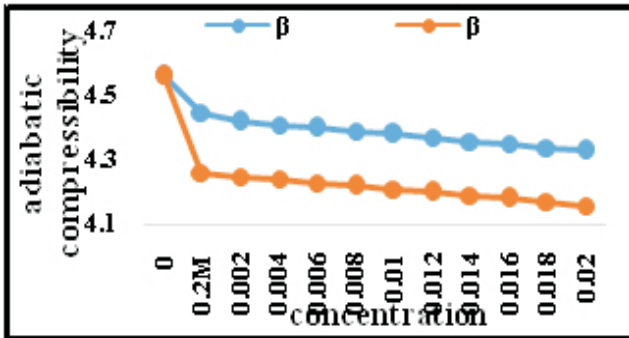


Fig. 3. Adiabatic compressibility versus concentration at 293.15K temperature.

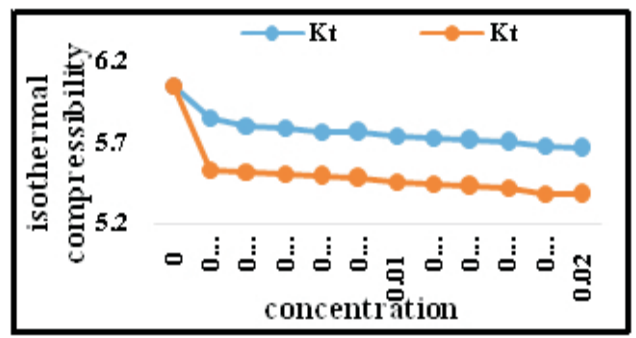


Fig. 8. Isothermal Compressibility versus concentration at 293.15K temperature.

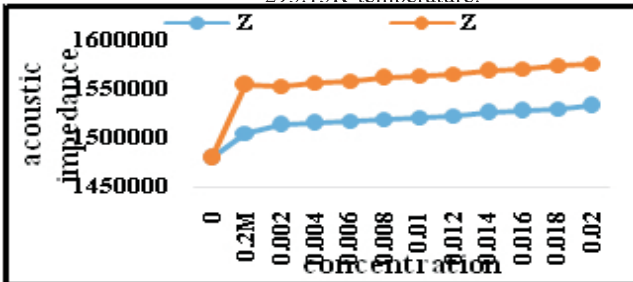


Fig. 4. Acoustic impedance versus concentration at 293.15K temperature.

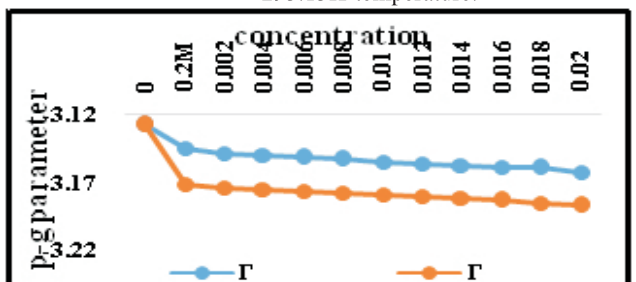


Fig. 8. Isothermal Compressibility versus concentration at 293.15K temperature.

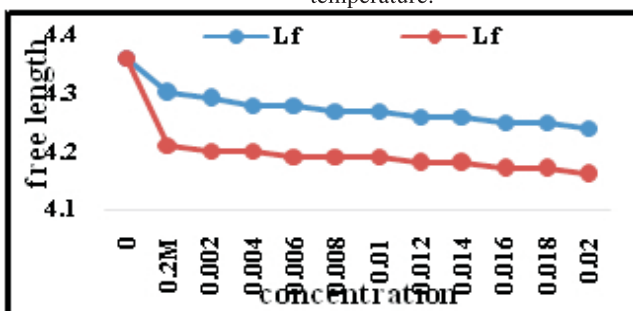


Fig. 5. Intermolecular free length versus concentration at 293.15K temperature.

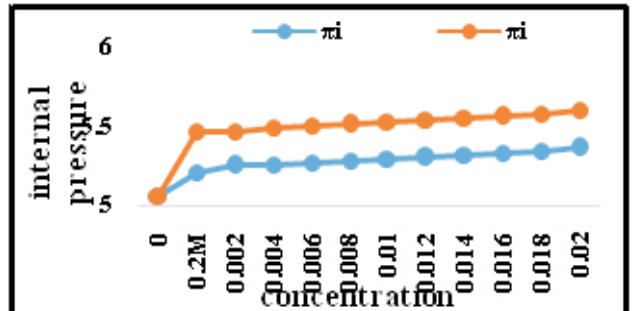


Fig. 10. Internal Pressure versus concentration at 293.15K temperature.

against the fertilizer concentration at a constant 293.15K temperature (Fig. 9). It is observed that the Pseudo-Grüneisen parameter values were negative and showed an increasing trend of variation with the addition of fertilizer in the saline salt solvent. The negative values suggests the probable formation of intermolecular complex in the system and strong intermolecular interaction. Pandey *et al.* (2006) also reported this kind of results in their research work and exposed the behavior of liquid and kind of interaction exist in that liquid.

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