Comparative Study of Molecular Interactions of Refined and Unrefined Soybean Oil and Unrefined Soybean Oil with Different Organic Solvents

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Abstract: The manufacture of food products is a highly dynamic and intensely competitive industry. The use of ultrasonic is an analytical technique for providing information about the physicochemical properties of foods is becoming increasingly popular in the food industry. Solvent extraction of oils is a common operation in the processing of seeds to obtain edible oils. The molecular interaction studies on oils and oil mixtures with organic solvents are becoming important in recent years because their properties are needed in food technology and oil industries. The present study focuses on the nature of intermolecular interactions existing between soybean oil and organic solvents using ultrasound. This paper presents data of ultrasonic velocities and densities of mixtures enclosing soybean oil and different solvents such as ethanol, 2-propanol, n-hexane and n-butyl acetate that have been measured over the entire range of composition at different temperatures i.e. 303K to 318K in the interval of 5K. The acoustical parameters namely adiabatic compressibility and relaxation time of the binary mixtures are calculated.

Keywords: Soybean oil, organic solvents, ultrasonic velocity, density, adiabatic compressibility and relaxation time

1. Introduction

The study of ultrasonic dispersion in liquids provides valuable information about their physicochemical properties. The molecular interaction studies on oils and with their organic solvents are becoming important in recent years because their properties are needed in food technology and oil industries. The thermo acoustical properties are given details regarding molecular forces acting between the molecules of the same substance in the pure liquids and molecules of different substances in the liquid mixtures. Soybean oil has been used as edible oil for thousands of years.

2. Methodology

All solvents used in the preparation of samples were of a purity greater than 99.0 mol%. The density is measured by relative density method using 10 ml relative density bottle with an accuracy of 0.001kg/m³. The measurements are made at 303 to 318K with the help of digitally controlled temperature bath was maintained constant using a thermostatically-controlled water circulating arrangement with an accuracy of ±0.1K. Density measurements were performed using density bottle. Masses were measured by a single pan electronic balance with an accuracy of ±0.1 mg. Ultrasonic velocity were measured by a MHF-400 high frequency pulser-receiver at a frequencies of 2MHz with an accuracy of ±0.1 m/s.

3. Results and Discussion

Ultrasonic velocity (u) is decreases with increase in temperature of refined soybean oil, unrefined soybean oil, unrefined soybean oil with ethanol, 2-propanol, n-hexane and n-butyl acetate. Figure 1 shows the variation of ultrasonic velocity (u) with temperature (K) of refined and unrefined soybean oil and unrefined soybean oil with their chemical additives at 2MHz frequency, from these, it can be noticed that velocities in all the oil and with their additives decreases with increase in temperature. This is further supported by an idea that sound wave travels faster in the close-packed arrangement of atoms than the loose-packed arrangement of atoms. This is in agreement with the theoretical prediction of velocity variation with temperature in high viscous oils. In refined and unrefined soybean oil and with their chemical additives, the velocity variation with temperature is approximately linear. These observations clearly indicate that the motion of sound wave largely depends on internal molecular dynamics in each oil and with their chemical additives. It may be indication for the existence of stronger intermolecular interactions between the triglyceride molecules soybean oil compared to the unrefined oil with chemical additives under considerations. Strong intermolecular interactions are expected due to the presence of hydroxyl (OH) groups within the fatty acid chains in unrefined soybean oil.

The differences observed the ultrasonic velocity decreases as the temperature increase for refined soybean oil, unrefined soybean oil and unrefined soybean oil + chemical additives. As expected, unrefined soybean oil shows the higher ultrasonic velocity, the system varies in the order unrefined
soybean oil > alkanols > acetate (ester) > alkanes > refined soybean oil. This trend is analogous to the ultrasonic velocity, where the maximum values are those of unrefined soybean oil and lowest, refined soybean oil. It is worthwhile to point out that the strong decreasing trend is in accordance with the self associative tendency oils with chemical additives at higher temperature. The effect of temperature on this parameter is slight but decrease in value when the temperature is increase.

The addition of solvents to soybean oil tends to cause breaking of disperse interactions and creation of better packed cluster with a consequent decrease in ultrasonic velocity and density and then, the corresponding increase in adiabatic compressibility. This important change of chemical environment is noted by a large and sharp modification of each acoustic parameter at infinite dilution of oil.

Density ($\rho$) is decreases with increase in temperature of refined soybean oil, unrefined soybean oil, unrefined soybean oil with ethanol, 2-propanol, n-hexane and n-butyl acetate. Figure 2 show the variation of density ($\rho$) with temperature (K) of refined and unrefined soybean oil and with their chemical additives. Density of the refined soybean oil, unrefined soybean, and unrefined soybean oil with their additives decreases monotonically and almost linearly with increase in temperature and this is in agreement with others observations. Within the experimental range of temperature, the densities of refined soybean oil and unrefined soybean oil with their additives were measured to be smaller than those of unrefined soybean oil where refined soybean oil and unrefined soybean oil with their additives was found to be denser than unrefined oils.

The variation of the adiabatic compressibility ($\beta_a$) is increases with increase in temperature of refined soybean oil, unrefined soybean oil, unrefined soybean oil with ethanol, 2-propanol, n-hexane and n-butyl acetate. Figure 3 shows the variation of adiabatic compressibility ($\beta_a$) with temperature (K) of refined and unrefined soybean oils and with different organic solvents. Adiabatic compressibility of the refined and unrefined soybean oil, unrefined soybean oil with their chemical additives increases with increase in temperature this indicates that the availability of large space in triglyceride molecules and triglyceride molecule with the second component of the binary mixtures and the impedance follows the opposite trend of compressibility decreasing with the molar concentration of solvents. This implies that, large space is available for the triglyceride molecules and mixtures to be compressed. Rising adiabatic compressibility suggest that triglyceride molecules are displaced by increasing organic solvents in the mixture. The differences observed in the adiabatic compressibility at finite dilution for each alcohol are due to variation in the hindrance of residue. As expected, unrefined soybean oil with n-hexane gives high adiabatic compressibility with increase in temperature. Increase in adiabatic compressibility of n-hexane with oil indicates that there is definite repulsion in the molecules and it also brings the molecules to a loose packing structure resulting into increase in intermolecular free length.

Figure 1: Variation of ultrasonic velocity with temp. (R. & UR. Soybean oil, UR. Soybean oil + Ethanol, 2-Propanol, n-Hexane, n-BA)

Figure 2: Variation of density with temp. (R. & UR. Soybean oil, UR. Soybean oil + Ethanol, 2-Propanol, n-Hexane, n-BA)

Figure 3: Variation of adiabatic compressibility with temp. (R. & UR. Soybean oil, UR. Soybean oil + Ethanol, 2-Propanol, n-Hexane, n-BA)

Figure 4: Variation of relaxation time with temp. (R. & UR. Soybean oil, UR. Soybean oil + Ethanol, 2-Propanol, n-Hexane, n-BA)
The increase in adiabatic compressibility also indicates that the enhancement of degree of dissociation in the molecules of the component liquid materials. Hence the intermolecular distance increases with increase in temperature. It is primarily the compressibility that changes with structure which leads to change in ultrasonic velocity.

Relaxation time (τ) is decreases with increase in temperature of refined soybean oil, unrefined soybean oil, unrefined soybean oil with ethanol, 2-propanol, n-hexane and n-butyl acetate. Figure 4 show the variation of relaxation time (τ) with temperature (K) of refined and unrefined soybean oils and with their chemical additives. Relaxation time is decreases with increase in temperature this indicates that the weak interactions in the triglyceride molecules and the values of the mixtures, thus confirming the presence of weak interaction in triglyceride molecules and in oil with solvents.

In this system adiabatic compressibility play very important role for decreasing relaxation time with increasing molar concentration. This indicates that the solution generally absorbs less ultrasonic energy.

Decrease in relaxation time of n-butyl acetate in unrefined oils with increase in temperature is caused by the energy transfer between translational and vibrational degrees of freedom and all these degrees take part in the processed observed. The dispersion of the ultrasonic velocity in the system should contain information about the characteristic time of the relaxation process that causes dispersion. The relaxation time which is in the order of $10^{-12}$ sec is due to structural relaxation process and in such a situation it is suggested that the molecules get rearranged due to cooperative process.

4. Conclusions

The addition of solvents in soybean oil tends to cause breaking of disperse interactions and the creations of better packed clusters with a consequent decrease in ultrasonic velocity and density and then, the corresponding increase in adiabatic compressibility. This important change in chemical environment is noted by a large and sharp modification of each acoustic parameter at infinite dilution of oil. Alcohol are polar and associating fluids and oils are esters, which are polar and non associating molecules. One possible explanation for the experimental results is that the strong hydrogen bonding effect between the alcohol molecules is disrupted in the binary mixture with esters.

References