

FINAL REPORT

PROJECT TITLE

MOLECULAR INTERACTION STUDIES IN BINARY LIQUID MIXTURES USING ULTRASONIC TECHNIQUES

Dr. S. G. Goswami

(Principal Investigator)

Recently Khasare derived an equation of state for L-J fluid by modifying an expression for work done, obtained from partition function through perturbation approach. This is achieved by inserting at some fixed position in the m-component fluid, a single solute particle of radius 'R' in n-dimensions along with the necessary thermodynamic requirements. It was therefore thought worthwhile to undertake a comprehensive investigation of Khasare's equation of state for real fluid as regards its applicability to various real fluids mixtures and capacity to predict thermodynamic behaviour in them. The theory has been applied to such binary liquid mixture systems which consists of different spatial arrangements of hard spheres solutes or solvent molecules at the same time are either polar or non-polar molecules in different environments.

In this project, the molecular interaction, dipole-dipole interaction, collision factors and hydrogen bond forces in binary systems containing at different temperature. The binary liquids systems under investigation are,

- Benzene in P-dioxane
- Benzene in methylcyclohexane
- Benzene in methylalcohol

The computational of ultrasonic velocity (u), density (ρ), depth of minimum potential for the mixtures ($\beta\epsilon_{AB}$), depth of minimum potential of liquid component of liquid A in presence of liquid component B ($\beta\epsilon_{AA}$), the depth of minimum potential of liquid component B in presence of liquid component A ($\beta\epsilon_{BB}$), the hard sphere diameter of liquid component A in presence of liquid component B (σ_{AA}) the hard sphere diameter of liquid component B in presence of liquid component A (σ_{BB}) and packing fraction (η) at temperature 303.15K employing the khasare's theory (on the basis of model equation of state of fluid mixtures for the respective binary liquid mixtures system)

Experimental Details

The experimental data evolved in the laboratory was used for the present theoretical investigation. The liquid of benzene, cyclohexane, methylcyclohexane and methyl alcohol were analar grade & redistilled before use. The binary mixture of different mole fraction of two components in system benzene -p-dioxane, benzene – methylcyclohexane, benzene-cyclohexanol were prepared immediately before use. The velocity of ultrasonic waves (u) at a frequency of 2MHz and density (ρ) in these binary liquids mixtures were measured by employing Ultrasonic interferometer and the hydrostatic sinker method in the temperature range 10-40°C and ultra Thermostate U-10 min of the samples constant to 0.1°C. The accuracy of one part in 10^4 in the velocity and one part in 10^4 in the density measurement is achieved. The variation of u and ρ in these mixtures were found to be linear with the temperature and hence method of least squares was applied and the values of u and ρ at different temperatures were calculated from the equation

$$u = u_0 + \left(\frac{du}{dT} \right)_{T=0} \cdot T, \quad \rho = \rho_0 + \left(\frac{d\rho}{dT} \right)_{T=0} \cdot T$$

Results of theoretical investigation

Benzene + p-dioxane

The variation of $\beta\epsilon_{AB}$ and η versus C_m of p-dioxane in benzene show constant increases of these parameters. Both the variations are almost identical. This observed increasing $\beta\epsilon_{AB}$ and η with C_m of p-dioxane shows presence of molecular interaction in these mixtures. Benzene is considered to be very weakly associative liquid (almost normal) and p-dioxane is known to give strong interactions with associative liquids. A weak associative molecular interaction is therefore expected between p-dioxane and benzene. On the other hand, this is also seen from the $\beta\epsilon_{AB}$, η , $\beta\epsilon_{AA}$, $\beta\epsilon_{BB}$, σ_{AA} , σ_{BB} (fig 1 - 3)

Benzene+ methylcyclohexane and Benzene + cyclohexanol

The larger $\beta\epsilon_{AB}$, η , $\beta\epsilon_{AA}$, $\beta\epsilon_{BB}$, σ_{AA} and σ_{BB} variation in a mixture containing cyclohexanol than methylcyclohexane in benzene (fig 4-9) indicates a stronger molecular interaction in cyclohexanol mixture than that in methylcyclohexane mixture. The heteromolecular interaction is not due to specific process, such as H-bonding or lone pair interaction, but is a ring – ring interaction. The larger size methyl group in methylcyclohexane would prohibit a closer approach between two rings in benzene- methylcyclohexane, resulting in a weak molecular interaction.

