COMPARATIVE ANALYSIS OF EXPERIMENTAL AND NUMERICAL INVESTIGATION ON THERMOPHYSICALPROPERTIES IN HYDRO CARBON MIXTURES USING JOUYBAN-ACREE MODEL AT VARIOUS TEMPERATURES

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ABSTRACT

The thermophysical properties of liquid mixtures provide additional information regarding molecular interactions. A perusal of the literature revealed that the predictions of thermophysical properties of liquid mixtures are scarce. With an aim, the thermophysical properties of viscosity, excess molar volume V^E and viscosity deviations $\Delta\eta$ of liquid mixtures are predicted by using various nonlinear models. In this reseach Jouyban-Acree viscosity models have been used for predicting viscosity of Acetophenone with P-xylene and 1, 4 Dioxane with Benzene at different mole fractions measured at various temperatures in the atmospheric pressure condition. From experimentation excess volumes, V^E, and deviations in viscosities, $\Delta\eta$, of mixtures at infinite dilutions have been obtained. The measured systems show positive V^E and negative $\Delta\eta$ with increasing temperatures. From the positive excess molar volume, when aromatics, which exist in a highly associated form in the pure state, are mixed with polar solvents (ketones), the monomerization occurs and new specific interactions appear in the solution.The negative viscosity deviation depends on the size and shape of the molecules and molecular interactions. These measured data tailored to the Jouyban-Acree nonlinear models to derive the binary coefficients Jouyban-Acree model is more adequate for the thermo physical and the standard deviation was found to be < 2.06 %. The molecular interactions existing between the components and comparison of liquid mixtures were also discussed.

Keywords: Acetophenone · 1, 4 Dioxane · Viscosity measurement · Jouyban-Acree Model ·

INTRODUCTION

The quantitative viscosity and density data of liquid mixtures are required to solve many engineering problems, involve in chemical separations, heat transfer, mass transfer, and fluid flow are important from practical and theoretical points of view, for understanding liquid theory. The low polarity of 1, 4 Dioxane is interesting to study with hydrocarbon mixtures, for the type of interaction between the components of binary systems.1,4 Dioxane commonly known as excellent aprotic solvent, it has a zero dipole movement and cyclic ether, that has an electron donor ability towards aromatic rings, it act like weak electron acceptors. 1, 4 Dioxane is used as a stabilizer in aluminium containers and solvent in inks and adhesives. There are few reports on density and viscosity data of 1, 4 Dioxane with hydrocarbon mixtures (Martin, 2001 and Ramesh et al., 2014). In our earlier paper, we had studied thermo physical properties of binary systems (Ramesh et al.,2014) . In the present paper, it has been reported density (ρ) and viscosity (η) of pure 1, 4 Dioxane, Acetophenone, P-xylene and Benzene for the binary system constituted by these two chemicals at entire range of composition and temperature 303.15K to 313.15K. With this data, the excess molar volume and deviation in viscosity have been computed. These results have been fitted to the Jouyban-Acree models and polynomial equations. The Jouyban-Acree model was used to correlate the viscosity and deviations in viscosities, $\Delta\eta$, this analysis technique was used to derive the binary coefficients, estimated the standard deviation (σ) between the experimental and calculated data (Jouyban et al., 2005). The variation of these parameters with the composition and temperature of the mixtures has been discussed in terms of the molecular interactions in these mixtures. The effect of the number and position of the methyl groups in these aromatic hydrocarbons on molecular interactions in these mixtures has also been discussed. A literature search showed that no measurements have been previously reported by using Jouyban-Acree models for the mixtures studied in this paper.

EXPERIMENTAL SECTION

Materials

1, 4-Dioxane, Acetophenone, P-xylene and Benzene this were all supplied by Merck Ltd. With the stated purities better than 99‰, were stored over molecular sieves (0.3 nm). To minimize the contact of these reagents with moist air, the products were kept in sealed bottles in a desiccator. The densities and viscosities of pure substances and experimental values comparison with literature values are listed in Table1(Martin, 2001, Ramesh et al., 2014, Jouyban et al.,2005, Baskaran, 2012, Laura, 2012 and Redlich, 194) .