EXPERIMENTAL AND NUMERICAL INVESTIGATION ON THERMOPHYSICAL PROPERTIES OF LIQUID MIXTURES USING JOUYBAN-ACREE MODEL AT VARIOUS TEMPERATURES

[1]M.GOKULAKRISHNAN, [2]K.SARAVANAKUMAR, [3]BRIJESH, [4]R.SENTHILKUMAR, [5]L.GOVINDARAJAN

[1]Department of Biotechnology, M. S.Ramaiah Institute of Technology, Bengaluru, India.
[2,4,5]Engineering Department, College of Applied Sciences, Sohar, MoHE, Sultanate of Oman
[3]Department of Chemical Engineering, M. S.Ramaiah Institute of Technology, Bengaluru, India
E-mail: [1]gokulsm@gmail.com, saroosaroo@gmail.com

Abstract- In this work, the physical properties of binary mixtures of Acetophenone with hexylbutyrate were measured. Densities and viscosities of the binary mixtures of Acetophenone with hexylbutyrate were measured at temperature ranging from 303.15 to 323.15 k over the entire range of mole fractions. The experimentally determined thermophysical properties of the binary liquid mixtures were used to calculate the excess molar volume and viscosity deviations with Acetophenone and hexylbutyrate liquid mixtures. The measured values of viscosity and density were fitted to the Jouyban – Acree model. It was found that in all cases, the data obtained fitted with the values correlated by the corresponding model precise well. The outcomes are interpreted in terms of molecular interactions occurring in the solution.

Keywords- Viscosity, Density, Thermophysical Properties, Liquid Mixtures, Molar Volume

I. INTRODUCTION

Viscosity and density is a prime thermophysical property of a compound which is very necessary in the study of fluids [1]. The studies of thermodynamics and transport properties of binary liquid mixtures contribute to the perception of the intermolecular interactions existing between the various species in a solution [2]. Information about the viscosity and density of mixtures and their dependence with composition is important in different surface facilities as well as for several other applications [3]. Thermodynamic studies also provide information about changes with respect to composition and filling efficiencies that take place in a solution through mixing processes [2]. The properties of binary mixtures are complex because they do not only depend on solute-solvent interactions, but also on the structural effects arising from interstitial properties from the differences in molar volume and free volume between components present in the solution [4]. Studies of mixtures of Acetophenone with other solvents are interesting for a number of scientific reasons connected with the formulation of testing models for the prediction of properties associated with fluids [2]. Acetophenone is a vital manufacturing chemical used as an ingredient of flavour and fragrance in soaps, detergents, cosmetics and perfumes. It has also been used as an important intermediate for pharmaceuticals and agrochemicals.

II. MATERIALS AND PROCEDURES

Acetophenone of reported purity 99.5%, and hexylbutyrate with reported purities of 99.5%, were obtained from Loba chemicals, dried over anhydrous calcium chloride, and then fractionally distilled before use. The purity of the solvents, after purification, was ascertained by comparing their densities and viscosities with the corresponding literature values at 303.15 K (Table 1). Binary mixtures were prepared gravimetrically using a Shimadzu Corporation (Japan) type BL 2205 electronic balance with an uncertainty of 0.01 g. Care was taken to avoid evaporation and contamination during mixing. The resulting mole fraction uncertainties were estimated to be less than ±0.0001. All of the measurements described below were performed at least three times and the presented results are their averages. The viscosity and density of the compounds and binary mixtures were measured using an Anton Paar SVM 3000 Stabinger viscometer and Anton Paar DSA 5000 density. For this device, two or more samples of each individual liquid or liquid mixture were measured at three temperatures between (303.15 and 323.15) K, and these replicates were used to determine the precision of the measurement.

Table 1 Comparison of experimental densities and viscosities of pure liquids with literature values at 303.15 K and 0.1 MPa

Pure Liquids	Density ρ/g·cm^{-3}		Viscosity η/(mPa·s)	
	Lit	Exp	Lit	Exp
Acetophenone	1.0194 [5,7]	1.0199	1.5130 [5,7]	1.5338
Hexyl butyrate	0.8465[6]	0.8467	1.310[6]	1.1317

III. RESULTS AND DISCUSSION

Experimental density (ρ), and viscosity (η), at temperatures of (303.15, 313.15 and 323.15 K) are

presented in Table 2. To investigate the molecular interactions between Acetophenone and hexylbutyrate, viscosity deviation, ($\Delta\eta$) and excess molar volumes VE, have been evaluated from experimental density and viscosity using the equations (1) and (2), respectively and also presented in Table 2.

$$V^E=(x_1M_1+x_2M_2)/\rho_m-(x_1M_1/\rho_1+x_2M_2/\rho_2) \quad (1)$$

where x_1 and x_2 refer to the mole fraction of components 1 and 2. ρ_1, ρ_2, and ρ_m refer to the density of components 1 and 2 and the density of the mixture, respectively. The viscosity deviations $\Delta\eta$ were calculated from the viscosity values using

$$\Delta\eta = \eta - (x_1\eta_1 + x_2\eta_2) \quad (2)$$

Table2. Experimental values of density ρ (g/cm^3), viscosity η (mPa·s), deviation in viscosity $\Delta\eta$ (mPa·s), excess molar volumes VE (cm^3 /mol)

Acetophenone (1) + hexylbutyrate (2)						
	ρ g·cm^{-3}			η/ (mPa·s)		
x_1	303.15	313.15	323.15	303.15	313.15	323.15
0.0000	0.8467	0.8372	0.8306	1.1317	0.9607	0.8246
0.1592	0.8640	0.8546	0.8475	1.1799	0.9964	0.8707
0.2987	0.8813	0.8720	0.8644	1.2238	1.0321	0.9178
0.4220	0.8986	0.8894	0.8813	1.2660	1.0677	0.9649
0.5318	0.9159	0.9068	0.8981	1.3061	1.1034	1.0112
0.6301	0.9333	0.9242	0.9150	1.3462	1.1391	1.0581
0.7187	0.9506	0.9416	0.9318	1.3860	1.1748	1.1031
0.7990	0.9679	0.9590	0.9486	1.4262	1.2105	1.1472
0.8720	0.9852	0.9764	0.9653	1.4646	1.2461	1.1933
0.9388	1.0025	0.9938	0.9820	1.4998	1.2818	1.2394
1.0000	1.0199	1.0112	0.9987	1.5338	1.3175	1.2855

	ρ / g ·cm-3.			η/ mPa·s		
K	303.15	313.15	323.15	303.15	313.15	323.15
A0	55.993	58.485	57.826	29.959	82.832	105.96
A1	5.5998	5.8313	5.595	6.8645	7.1751	6.5398
A2	-36.55	-38.176	-37.59	-10.80	-53.50	-73.91
A3	-8.613	-8.9776	-8.727	-8.502	-11.52	-11.71
A4	-21.86	-22.844	-22.76	-20.57	-32.85	-36.18
S	0.0001	0.0006	0.0004	0.0005	0.0006	0.0005

Table.3 Parameters and standard deviations of Jouyban- Acree model for Acetophenone (1) + hexylbutyrate (2) mixture

Jouyban et.al [7] proposed a model for correlating the thermal properties of liquid mixtures at various temperatures

$$\ln \eta_{m,T} = x_1 \ln \eta_{1,T} + x_2 \ln \eta_{2,T} + A_0 (x_1x_2/T) + A_1[(x_1x_2(x1\text{-}x2)/T)] + A_2[(x_1x_2(x_1\text{-}x_2)^2/T)] + A_3[(x_1x_2(x_1\text{-}x_2)^3/T)] \quad (4)$$

where $\eta_{1,T}$ and $\eta_{2,T}$ are viscosity of pure liquids at temperature T and A_0- A_3 are the model constants. These constants are computed by a least squares analysis.

In each case, the optimum number of coefficients is ascertained from an examination of the variation in standard deviation (S). S was calculated using the relation

$$S(Y)=[\Sigma(Aexp-Acal)2/(N-n)]½ \quad (3)$$

where N is the number of data points and n is the number of coefficients. The calculated values of coefficients along with the standard deviation (S) are given in Table 3.

The variation of excess volumes with the mole fraction (x1) of acetophenone and hexylbutyrate at (303.15, 313.15 and 323.15) K are represented in figure1. This shows that the excess molar volumes are always negative for all the studied temperatures. Treszczanowicz et al.[9] and Roux and Desnoyers[10] suggested that VE is the resultant contribution from several opposing effects. These may be divided arbitrarily into three types, namely chemical, physical and structural. A physical contribution that is specific interactions between the real species present in the mixture, contribute a negative term to VE. The chemical or specific intermolecular interactions result in a volume decrease and these include charge transfer type forces and other complex forming interactions. This effect contributes negative values to VE. The structural contributions are mostly negative and arise from several effects, especially from interstitial accommodation and changes of free volume. In other words, structural contributions arising from geometrical fitting of one component into the other due to the differences in the free volume and molar volume between components lead to a negative contribution to VE.

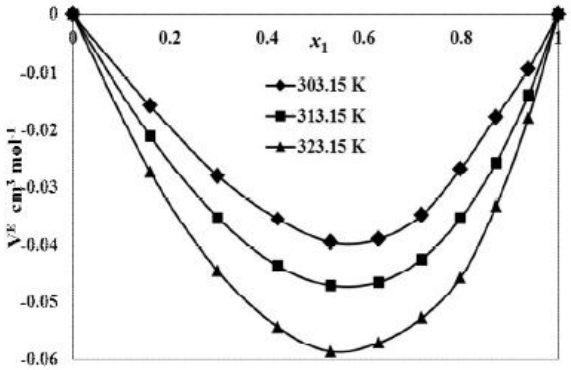


Figure 1. Excess Molar Volume, V^E, for the system Acetophenone (1) + Hexylbutyrate (2) at temperatures: ▲,T= 303.15 K; ■,T= 313.15 K; ▲,T= 323.15 K

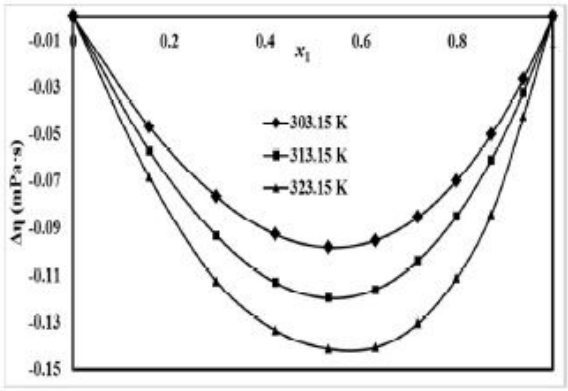


Figure 2. Viscosity deviation„ for the system Acetophenone (1) + Hexylbutyrate (2) at temperatures: ▲,T= 303.15 K;■,T= 313.15 K;▲,T= 323.15 K

The negative deviation in viscosity (Fig. 2) over the whole composition range for all mixtures decreases in absolute value as the temperature is increased, due to weakening of interaction. This negative deviation suggests that in these mixtures, the forces between unlike molecules are lesser than the forces between like molecules [11, 12].

CONCLUSIONS

Densities and viscosities for binary mixtures have been measured. The interactions between the liquids in liquid mixtures under investigation are either strong specific type or weak dispersive type interactions. Excess molar volumes and viscosity deviations of acetophenone and hexylbutyrate were obtained from the experimental results and fitted by Jouyban – Acree viscosity model. Jouyban – Acree shows the standard deviation of <0.0005. Jouyban – Acree viscosity model holds good for the viscosity of binary liquid mixtures under investigation. Jouyban-Acree model is more adequate for the thermo physical properties of liquid mixtures. It has been concluded that the Jouyban - Acree model is very well suited for correlating the thermo physical properties of the binary mixture studied.

REFERENCES

[1] Kim E S & Marsh K N, J Chem Eng Data, 33 (1988) 288.
[2] Mchaweh A, Alsaygh A & Mosh-Feghian M A, Fluid Phase Equilib, 224 (2004) 157.
[3] Kenart C M & Kenart W, Phys Chem Liq, 38(2000)155.
[4] T. G. Lavanya K. Saravanakumar · R. Baskaran · T. R. Kubendran, Int J Thermophys (2013) 34:1280–1287.
[5] K. Saravanakumar, T. G. Lavanya, R. Baskaran & T. R. Kubendran, J Iran Chem Soc (2012) 9:277–283.
[6] K. Saravanakumar, R. Baskaran , T.R. Kubendran, J Solution Chem (2011) 40:955–967
[7] B R. Ramesh, M.Gokulakrishnan, K. Saravanakumar, Journal of Engineering Thermophysics 25 (2), 227-235
[8] Jouyban A, Khoubnasabjafari M, Vaezgharamaleki Z, Fekari Z & Jr.Acree W E, Chem Pharm Bull, 53(2005)519.
[9] Treszczanowicz A J, Kiyohara O & Benson G C, J Chem Thermodyn, 13(1981)253.
[10] Roux A & Desnoyers J, J Proc Chem Soc, 78(1978)435.
[11] K. Saravanakumar, T. G. Lavanya, R. Baskaran and T. R. Kubendran,Rus J Phy chem, 2012, vol. 86, № 4. 647–655
[12] TR Saravanakumar, K., Lavanya, T.G., Baskaran, R. and TR Kubendran, Russian Journal of Physical Chemistry-A 86 (4), 647-655

★★★