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THERMODYNAMIC STUDIES OF BINARY MIXTURE CONTAINING PALM OIL + N-HEXANE AT 298.15K.

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Abstract

The relative density of the pure components(n-hexane), Palm oil & mixtures containing two components (binary mixtures) of Palm oil with n-hexane were measured at temperatures 298.15, mole fractions from 0.1 to 0.9. Relative Densities were determined using Specific gravity bottle.By using experimental densities excess molar volumes of binary mixtures were determined. The calculated values of excess molar volumes were interlinked with Redlich- Kister polynomial expansions.The values of the molar excess volumes suggest that interactions between the two liquids get stronger up to certain mole fraction & then get weaker afterward.

Keywords: Relative Density; Excess molar volumes; Palm Oil; n-hexane.

Introduction:

In the last 10-20 years biofuel[1-2]hasattained much attention to be used as a substituentfuel due to hazardous environmental issues& thecontinuous consumption of the non-renewable energy resources. The biofuels are consisting of mixture of alkyl ester of long chain carboxylic acids."It can also be synthesized by homogeneous catalysis with a trans esterification reaction[3]". However the mixtures of diesel with biodiesel are circulated for commercial purpose in the diesel marketplace,even then there are challenges due to inter-molecular interactions between different molecules of diesel & biodiesel & their effect on thermodynamic properties[4]. So,our research group is going to provide a group of new experimental data on transport, density & aquired properties on biofuel-diesel & biofuel-biodiesel mixtures.The experimental value for the density & excess thermodynamic properties are very important in many industrial, chemical & biological processes, particularly for mixed systems, For example: optimization of combustion process & serving as input for simulation[1]. Further the excess thermodynamic properties are very useful in underst&ing of intermolecular interactions[2]. So, this research work is focused at calculating the density of binary of Palm oil + n-hexane at the temperature of 298.15 & at the atmospheric pressure, which is a function of composition. Excess molar volumes ,V^E, of binary mixturewere calculated by using density data.. Major data have been interlinked using Redlich-Kister type functions in terms of the mole fraction.As n-hexane, used in cooking oil hence it is used as a representative of fuel[6-7]. It must be noted that, as biodiesel have a complex composition hence it is presumed that the mixtures containing biodiesel are pseudo-binary mixtures[8] .

Materials & Methods

Palm Oil was supplied byBiod Chemicals, Rewari, INDIA (Purity = 99.9%). It was used without any further purification. "n-Hexane (Fluka, 99 mol%) was first treatedwith concentrated H_2SO_4, then with 0.1N solution of $KMnO_4$ in 10% H_2SO_4 & in last step with 0.1N solution of $KMnO_4$ in 10% sodium hydroxide, followed by washing with distilled water[9]".Methyl ester composition of Palm Oil was analyzed by GC-MS, at SAIF, Ch&igarh. In **Table 1**, the chemical composition is summarized."Binary mixtures were obtained by mixing the suitable volumes of liquid components in special glassware that have air tight Teflon coated caps[10,13-15]." The density of the mixture at specified temperature was measured on the same day after making mole fraction from 0.1 to 0.9 using specific gravity bottles. The variability in mole fraction is ±0.0001.

Table 1:Summarized data of Palm Oil using GC-MS

GC/MS Profile of Palm Oil

Compund name	RT	Molecular Formula	Cas #
Nonanoic acid, methly ester	17.04	$C_{10}H_{20}O_2$	1731-84-6
Tetradecanoic acid, 10, 13-dimethly-, methly ester	17.04	$C_{17}H_{34}O_2$	267650-23-7
Decanoic acid, 2-methly-	17.04	$C_{11}H_{22}O_2$	24323-23-7
Undecanoic acid, 2-methly-	17.04	$C_{12}H_{24}O_2$	24323-25-9
Dodecanoic acid, 2-methly-	17.04	$C_{13}H_{26}O_2$	2874-74-0

Results & Discussions:

The excess molar volumes (V^E) of pure liquids & mixtures were computed by using the experimental densities of pure liquids & their mixtures using the below equation[11]

$$V^E = \sum_{i=i}^{j} x_i M_i (\rho_{ij})^{-1} - \sum_{i=i}^{j} x_i M_i (\rho_i)^{-1} \quad (1)$$

ρ_{ij} is the density of binary mixture, x_i is mole fraction of Palm Oil in mixture & M_i is molecular mass of Palm Oil & n-hexane.

The excess molar volumes were correlated by Redlich – Kister[12] as shown in Eq. (2):

$$X^E (X = V) = x_i x_j [X^{(0)} + X^{(1)} (2x_i - 1) + X^{(2)} (2x_i - 1)^2] \quad (2)$$

where $X^n (X = V)$ (n=0-2) are the adjustable parameters & characteristics of (i + j)mixtures.

$$\sigma(X^E) = [\Sigma(X^E_{exptl} - X^E_{calc.Eq.(5)})^2 / (m - n)]^{0.5} \quad (3)$$

m & n represent the number of experimental points & parameters respectively.

The GC-MS profile ofpalm oilis reported in **Table 1**. From the table it is clear that the major component of Palm Oil is Tetradecanoic acid 10,13-dimethyl, methyl ester. The experimental density values for the pure components (n-hexane& Palm Oil) & for the binary mixture at 298.15K are summarized in **Table 2 & 3**respectively.

Table 2: Experimental densities for pure liquids at 298.15K & at atmospheric pressure.

Name of Liquid	Temperature	Density (g/cm^3)
Palm Oil	298.15K	0.8699
n-Hexane	298.15K	0.6548

Table 3: The Experimental densities for binary mixture (Palm oil (x_i) + n-hexane ($1 – x_i$)) at the temperature 298.15K

Palm oil (x_i) + n- Hexane ($1-x_i$) at 298.15 K

x_i	0.1013	0.2021	0.3012	0.4013	0.5011	0.6021	0.7001	0.8002	0.9016
Density (ρ) (g/cm^3)	0.7621	0.7711	0.7798	0.7812	0.7865	0.7901	0.8001	0.8112	0.8224

Table 4: The Excess molar volume of binary mixture (Palm oil (x_i)+ n-hexane ($1 – x_i$) at the temperature 298.15

Palm oil (x_i) + n- Hexane ($1-x_i$) at 298.15 K

x_i	0.1013	0.2021	0.3012	0.4013	0.5011	0.6021	0.7001	0.8002	0.9016
V^E	0.2113	0.1176	0.2246	0.2230	0.2085	0.1467	0.0412	0.0565	-0.1455

Table 5: Values of estimated parameters used for binary mixture along with st&ard deviation calculated using Eq. (2) & (3) :

T/K	X^0	X^1	X^{2-}	$\sigma/cm^3 \cdot mol^-$
293.15	0.8321	0.1447	-1.0967	0.2461

The variation of density & binary mixture is represented in figure 1 & 2

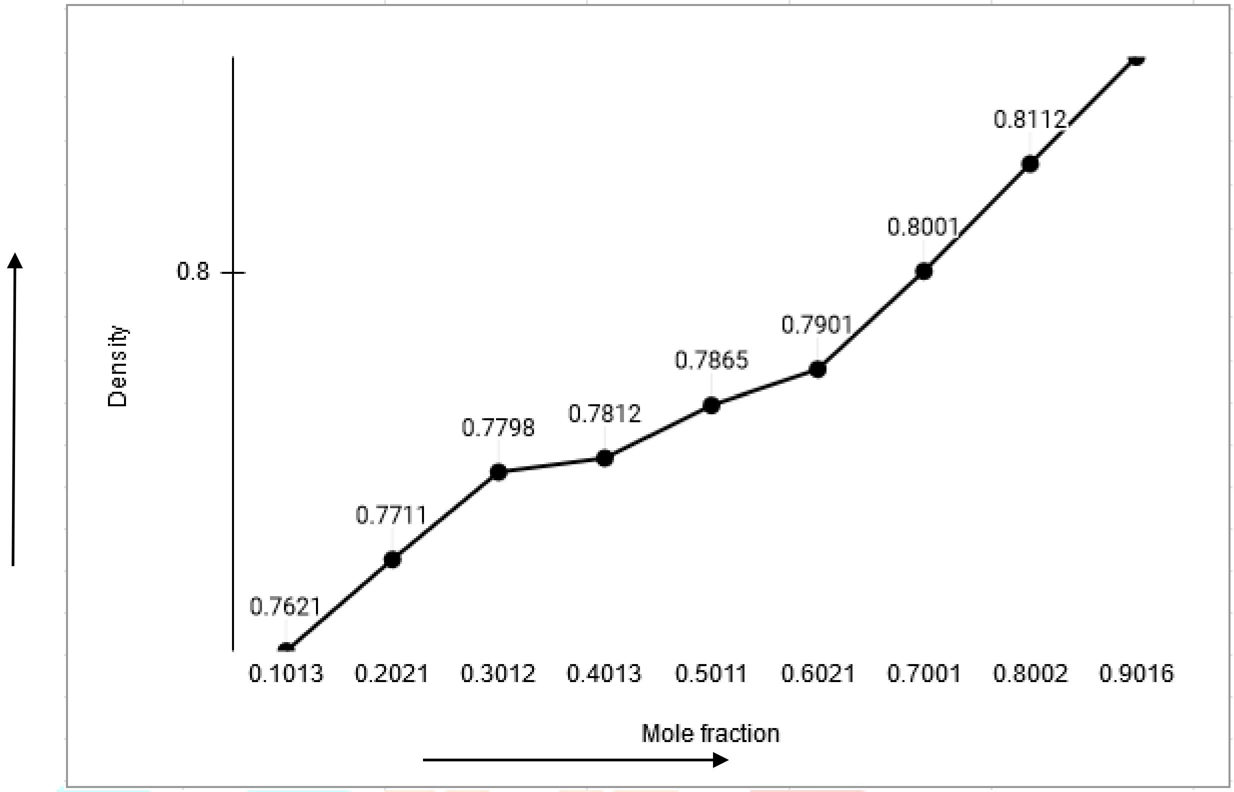

Figure1: Densities (ρ) for the binary mixture (Palm oil (x_i + n-hexane (1 – x_i)at the temperatures T=298.15K. Symbols represents the experimental points.

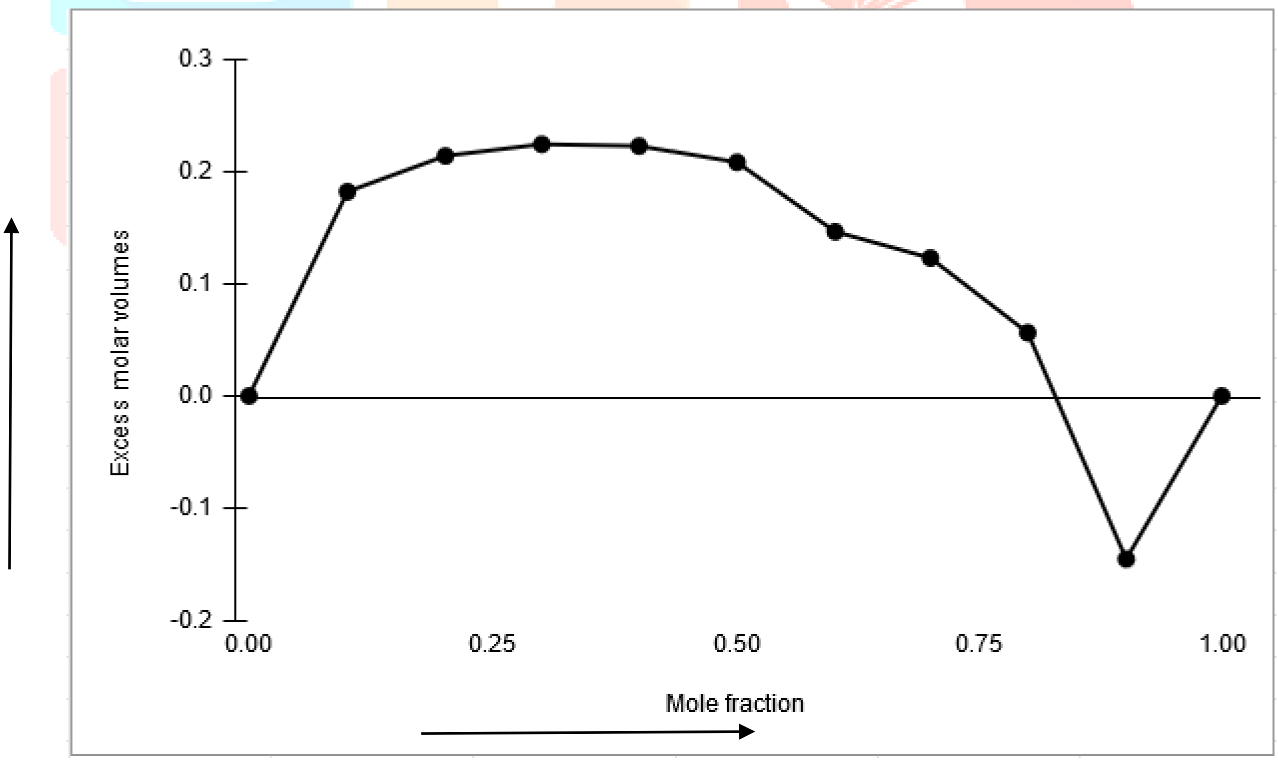

Figure 2: The Excess molar volumes for the binary mixtures (Palm oil (x_i)+ n-hexane (1 – x_i) at the temperature T=298.15. Symbols represents the experimental points.

Conclusions

The research work reports the experimental densities for the pure & binary mixture containing Palm Oil & n-hexane at 298.15K & atmospheric pressure. By using the values of densities of binary mixture excess molar volumes (V^E) were calculated. The values of excess molar volumes for the binary mixture at 298.15K are positive up to 0.8002 mole fraction & become negative at 0.9 mole fraction. This experimental VE data were interlinked satisfactorily by using Redlich- Kister equation. From the above data it can concluded that, usually, if the mole fraction of palm oil in mixture rises the intermolecular interactions get weakened.

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