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Prediction of Refractive index of binary mixture containing sunflower biodiesel and 3-methyl-1-butanol: experimental and theoretical interpretation

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ABSTRACT

Refractive index (*n*) of binary mixture containing sunflower biodiesel (S) and 3-methyl-1-butanol (3M1B) were measured at T = (298.15-318.15) K at 0.1 MPa over the entire composition range of mole fractions. The *n* values of pure compounds and its binary mixtures were measured by using refractometer (Anton Paar Abbemat 200). The *n* values have been measured in terms of different mixing rules like Lorentz-Lorentz (L.L), Gladstone-Dale (G.D), Heller-relation (H.R) and Weiner-relation (W.R). The experimental data of *n* compared well with the values obtained by using mixing rules for binary mixture S (1) + 3M1B (2). The measured data were correlated by Redlich-Kister polynomial equation. The effect of temperature has also been studied.

Keywords: Biodiesel; sunflower; refractive index; mixing rule

Introduction

The environmental problems caused by the continuous use and shortage of petroleum are encourage researchers to explore renewable energy resources. The most satisfactory alternate fuels are derivatives of vegetables oils i.e. Biodiesel [1]. Due to many of their applications and properties in different manners, researchers are attracting toward it and found interest in this work. These derivatives are renewable oxygenated and biodegradable fuel whose properties are very similar to diesel. The researchers are regularly in search for environment-friendly and alternative renewable energy sources [2-6]. The biodiesel can be obtained by transesterification in which alkyl group of an ester is replaced through interaction between the triacylglycerol of fats (oil) and an alcohol [7]. The common feedstock for production biodiesel can be sunflower, rapeseed, palm, soyabean and many other seed oils. Some of there thermo-physical properties are very similar to fossil fuels which recommend that it can be used without any modification in diesel engine. Still some problems have been noticed with use of biodiesel. The direct use of biodiesel and alcohols in diesel engine does not gives satisfactory effects on engine operation due to some limitations which promotes the blending and formation of binary mixtures [8]. The binary mixture of Biodiesel and alcohols helps to improve emission, performance and combustion. As pentanol and its isomers have better blend stability and miscibility and high energy density which helps to avoid the problems occur during blending with low carbon alcohols. Researchers have been working hard in recent years to develop new techniques. Researchers are continuously shows interest in the optical properties of biodiesels and alcohols mixtures for understanding the molecular systems and interactions in compounds, because thermo-physical properties plays an important role for scientific study and commercial process design [9, 10]. The study of thermo-physical properties plays an important role in understanding the molecular interaction in pure solution and liquid compounds [11-14]. In our present work the optical study of binary mixture containing sunflower biodiesel and 3-methyl-1-butanol is performed at different temperature range from 298.15-318.15 K. Various mixing rules like Lorentz-Lorentz (L.L), Gladstone-Dale (G.D), Heller-relation (H.R) and Weiner-relation (W.R). were used for the comparison with the predicted values. The data was best fitted and found to be in good agreement.

Experimental

Material and method

Sunflower biodiesel was supplied by Sun chem pvt ltd . 3 methyl -1 butanol of analytical grade was supplied by sigma Aldrich. The fatty acid composition of sunflower biodiesel was analysed by GC-MS profile. The experiment was performed on the refractometer (Anton Paar Abbemat 200) having temperature-controlled within $\pm 0.01\,\text{K}$. In accuracy in measurement of refractive index was $\pm 1\times 10^{-4}$. The readings for binary mixture were taken at different temperature ranging from 298.15 to 318.15 K at atmospheric pressure. All mole fractions of binary liquid mixtures were prepared by weigh. For measuring exact weight, airtight weighing bottle and OHAUS, AR224CN weighing balance was used. Weight of samples was measured by accuracy of ± 0.1mg. The resulted values of refractive index of all components at different temperature is well compared with literature values. Proper care was taken to avoid despoliation during mixture.

Results and Discussion

Refractive index

The Δn values were calculated for S (1) + 3M1B (2) by using n_D values in Eq. 1 and shown in table 1.

$$\Delta n = n_D - \sum_{i=1}^{2} x_i n_{Di} \qquad (1)$$

Where x_i represents the mole fractions, n_{Di} and n_D represents the n_D of pure components and its binary mixtures. Further Δn data were fitted to R.K. Eqn. (2) standard deviation σ and adjustable parameters $X^{(n)}$ are reported in Table S1.

The refractive index of the mixture containing sunflower biodiesels and 3M1B at different temperatures ranging from 298.15-318.15 K were measured over the entire mole fractions range.

Table 1. n_D and Δn for S (1) + 3M1B (2) at different temperature and 0.1 MPa pressure.

x_1	n_D	Δn	n_D	Δn	n_D	Δn	n_D	Δn	n_D	Δn
S (1) + 3M1B (2)										
298.15 K			303.15 K		308.15 K		313.15 K		318.15 K	
0.0995	1.4142	0.006	1.4122	0.006	1.4101	0.006	1.4081	0.006	1.4061	0.006
0.1250	1.4164	0.007	1.4143	0.007	1.4122	0.007	1.4102	0.007	1.4082	0.007
0.2124	1.4220	0.009	1.4200	0.009	1.4179	0.009	1.4158	0.009	1.4139	0.009
0.3320	1.4278	0.010	1.4257	0.010	1.4237	0.010	1.4216	0.010	1.4196	0.010
0.4323	1.4316	0.010	1.4295	0.010	1.4275	0.010	1.4253	0.010	1.4232	0.010
0.5284	1.4345	0.009	1.4325	0.009	1.4305	0.009	1.4285	0.009	1.4265	0.009

0.6441	1.4375	0.008	1.4357	0.008	1.4336	0.008	1.4315	0.008	1.4294	0.008
0.7444	1.4395	0.006	1.4375	0.006	1.4355	0.006	1.4334	0.006	1.4313	0.006
0.8358	1.4411	0.004	1.4391	0.004	1.4371	0.004	1.4350	0.004	1.4329	0.004
0.9086	1.4423	0.002	1.4403	0.002	1.4382	0.002	1.4362	0.002	1.4341	0.002

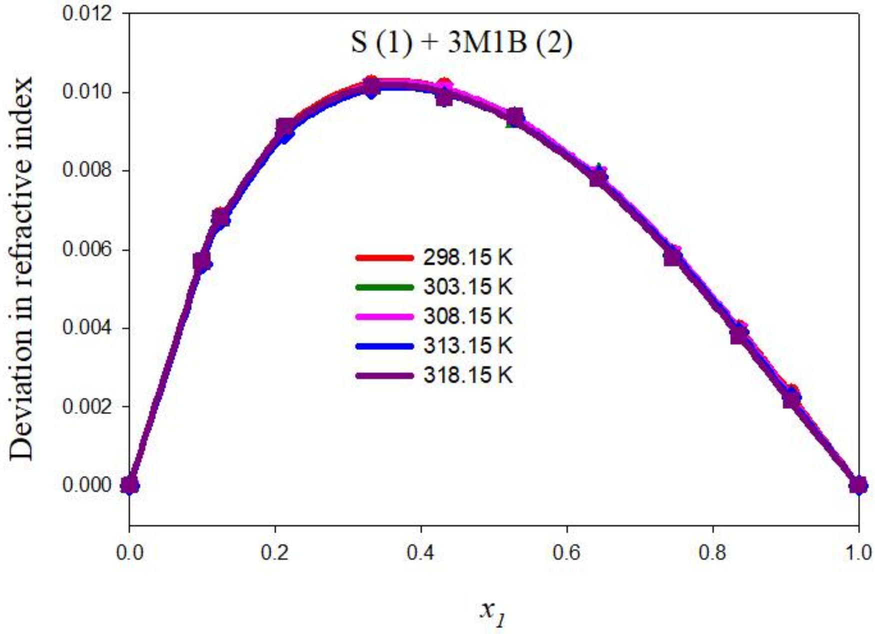

Figure 1. The Δn values of S (1) + 3M1B (2) at different temperature. solid line (R.K. Eq.), Symbol (expt.).

Further, Δn data were fitted to R.K. equation

$$X_m^E\left(X=\Delta n\right)=x_1x_2\left[\sum_{n=1}^{4}X^{(n)}\left(x_1-x_2\right)^{n-1}\right] \quad (2)$$

$$\sigma\left(X_m^E\right)=\left\{\frac{\sum\left(X_m^E(\exp tl.)-X_m^E(cal.)\right)^2}{(m-n)}\right\}^{1/2} \quad (3)$$

Where *n* represent the number of adjustable parameters and *m* represent the number of data point respectively.

The deviations in refractive index of the mixture containing sunflower biodiesel and 3M1B were measured over the entire range of mole fraction at different temperatures. Optical properties of matter depend upon speed of light in medium and it is proportional to density of medium.

The Δn shows positive values over the whole mole fraction range. Same trend is shown for all temperatures from 298.15k-318.15k. The positive values of refractive index are considered due to the presence of significant interactions in the mixture.

As the refractive index of binary or ternary mixtures were estimated from the pure components by using certain mixing rules [15-17]. Lorentz-Lorentz, gladstone-dale, weiner -relations, Heller -relation are most common used mixing rules.

Table 2. n_D **values using various correlations for P (1) + Alkanols (2) at different temperature.**

x_1	Exptl. (n_D)	G-D (n_D)	L-L (n_D)	W (n_D)	H (n_D)
S (1) + 3M1B (2)					
298.15 K					
0.0995	1.4142	1.4146	1.4145	1.4156	1.4144
0.1250	1.4164	1.4166	1.4165	1.4175	1.4165
0.2124	1.4220	1.4223	1.4222	1.4230	1.4222
0.3320	1.4278	1.4282	1.4281	1.4287	1.4281
0.4323	1.4316	1.4319	1.4318	1.4323	1.4319
0.5284	1.4345	1.4348	1.4347	1.4351	1.4348
0.6441	1.4375	1.4376	1.4375	1.4378	1.4376
0.7444	1.4395	1.4396	1.4396	1.4397	1.4396
0.8358	1.4411	1.4412	1.4411	1.4413	1.4412
0.9086	1.4423	1.4423	1.4423	1.4423	1.4423
303.15 K					
0.0995	1.4122	1.4126	1.4125	1.4136	1.4125
0.1250	1.4143	1.4146	1.4145	1.4155	1.4145
0.2124	1.4200	1.4204	1.4202	1.4211	1.4203
0.3320	1.4257	1.4262	1.4261	1.4268	1.4262
0.4323	1.4295	1.4300	1.4299	1.4304	1.4299
0.5284	1.4325	1.4329	1.4328	1.4332	1.4328
0.6441	1.4357	1.4357	1.4356	1.4359	1.4357
0.7444	1.4375	1.4377	1.4377	1.4378	1.4377
0.8358	1.4391	1.4393	1.4392	1.4393	1.4393
0.9086	1.4403	1.4404	1.4404	1.4404	1.4404
308.15 K					
0.0995	1.4101	1.4105	1.4104	1.4115	1.4104
0.1250	1.4122	1.4125	1.4124	1.4134	1.4124
0.2124	1.4179	1.4183	1.4181	1.4190	1.4182
0.3320	1.4237	1.4241	1.4240	1.4247	1.4241
0.4323	1.4275	1.4279	1.4278	1.4283	1.4278
0.5284	1.4305	1.4308	1.4307	1.4310	1.4307

0.6441	1.4336	1.4336	1.4335	1.4338	1.4336
0.7444	1.4355	1.4356	1.4356	1.4357	1.4356
0.8358	1.4371	1.4372	1.4371	1.4372	1.4372
0.9086	1.4382	1.4383	1.4383	1.4383	1.4383
313.15 K					
0.0995	1.4081	1.4085	1.4084	1.4095	1.4084
0.1250	1.4102	1.4105	1.4104	1.4114	1.4104
0.2124	1.4158	1.4163	1.4161	1.4170	1.4162
0.3320	1.4216	1.4221	1.4220	1.4226	1.4221
0.4323	1.4253	1.4259	1.4258	1.4263	1.4258
0.5284	1.4285	1.4288	1.4287	1.4290	1.4287
0.6441	1.4315	1.4316	1.4315	1.4318	1.4316
0.7444	1.4334	1.4336	1.4336	1.4337	1.4336
0.8358	1.4350	1.4352	1.4351	1.4352	1.4352
0.9086	1.4362	1.4363	1.4363	1.4363	1.4363
318.15 K					
0.0995	1.4061	1.4064	1.4063	1.4074	1.4063
0.1250	1.4082	1.4084	1.4083	1.4094	1.4083
0.2124	1.4139	1.4142	1.4141	1.4149	1.4141
0.3320	1.4196	1.4201	1.4200	1.4206	1.4200
0.4323	1.4232	1.4238	1.4237	1.4242	1.4238
0.5284	1.4265	1.4267	1.4266	1.4270	1.4267
0.6441	1.4294	1.4296	1.4295	1.4298	1.4295
0.7444	1.4313	1.4316	1.4315	1.4317	1.4316
0.8358	1.4329	1.4332	1.4331	1.4332	1.4332
0.9086	1.4341	1.4343	1.4343	1.4343	1.4343

For quantitative determination of n_D these different mixing rules were employed and shown in Fig.3.

Gladstone-Dale (G-D)

$$n_D - 1 = (n_{D1} - 1)\varphi_1 + (n_{D2} - 1)\varphi_2$$

Lorentz -Lorenz (L-L)

$$\frac{n_D^2 - 1}{n_D^2 + 2} = \left(\frac{n_{D1}^2 - 1}{n_{D1}^2 + 2}\right)\varphi_1 + \left(\frac{n_{D2}^2 - 1}{n_{D2}^2 + 2}\right)\varphi_2$$

Weiner (W)

$$\frac{n_D^2 - n_{D1}^2}{n_D^2 + 2n_{D2}^2} = \left(\frac{n_{D2}^2 - n_{D1}^2}{n_{D2}^2 + 2n_{D2}^2}\right)\varphi_2$$

Heller (H)

$$\frac{n_D - n_{D1}}{n_{D1}} = \frac{3}{2}\left(\frac{(n_{D2}/n_{D1})^2 - 1}{(n_{D2}/n_{D1})^2 + 2}\right)\varphi_2$$

In the above equations φ_1 and φ_2 are volume fraction and given by

$$\varphi_1 = \frac{x_1 V_1}{\sum x_i V_i} \quad \text{and} \quad \varphi_2 = \frac{x_2 V_2}{\sum x_i V_i}$$

Where V_i is the molar volume and x_i is the mole fraction of ith components. For these correlations n_D and standard deviation ($\sigma(\eta)$) were also calculated and shown in Table 2 & 3.

Table 3. Standard deviation $\sigma(\eta)$ in n_D using various correlations for P (1) + Alkanols (2) at different temperature.

Temperature	Gladstone-Dale	Lorentz -Lorenz	Weiner	Heller
298.15 K	0.0002	0.0001	0.0008	0.0002
303.15 K	0.0003	0.0002	0.0009	0.0003
308.15 K	0.0003	0.0002	0.0008	0.0002
313.15 K	0.0003	0.0002	0.0009	0.0003
318.15 K	0.0003	0.0002	0.0009	0.0003

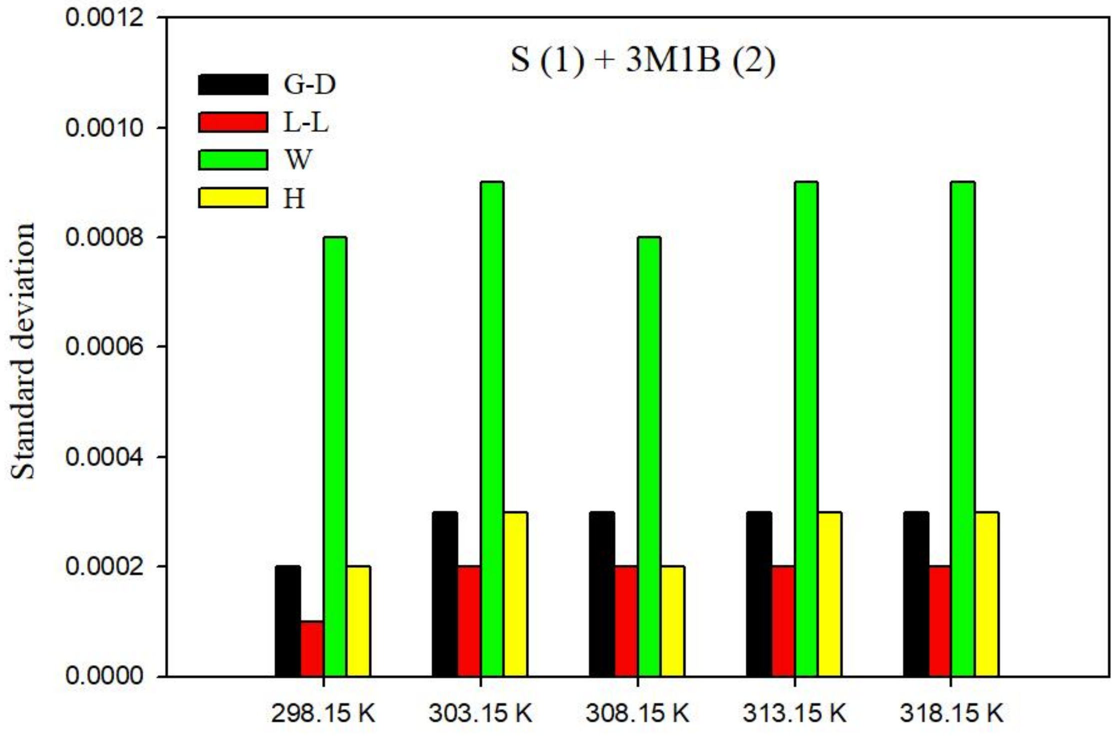

Figure 2. Standard deviation in n_D using various correlations at different temperature.

Conclusions

The *n* values of binary mixture containing S (1) + Alkanols (2) at T = 298.15-318.15 K at 0.1 MPa over the entire composition range of mole fractions are reporting . Further, the *n* values used to calculate the Δn . The Δn is found positive for all binary mixtures at whole compositions range. Δn follow the positive trend from temperature 298.15-318.15 k. The *n* values have been measured in terms of different mixing rules like Lorentz-Lorentz (L.L), Gladstone-Dale (G.D), Heller-relation (H.R) and Weiner-relation (W.R) .Also, the measured data were correlated by Redlich-Kister polynomial equation. Further Δn values were interpretate in term of intermolecular hydrogen bonding between S (1) + 3M1B mixture.

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