Numerical and Experimental Analysis of Optical Property of Polymers (PEG & PPG)

Gayathri A [#1], Venugopal T [*2],

[#]*Assistant Professor, Department of Mathematics, SCSVMV University, Kanchipuram – 631561, India*
** Director (Research & Publications), SCSVMV University, Kanchipuram – 631561, India*

***Abstract*—** *Refractive index plays a vital role in many branches of physics, chemistry and biology. In optics, the refractive index or index of refraction n of a material is a dimensionless number that describes how light propagates through that medium. Polymers are becoming increasingly attractive for a variety of optical applications such as lenses, optical circuits, optical fibers, anti-reflective films and coatings, optical adhesives, LCD displays, waveguides, UV-reactive inks and varnishes. There are many standard mathematical methods available to measure the Refractive Index. In the present study, Abbe refractometer is used for experimental measurement of refractive Index. In this paper, the refractive index of Polypropylene Glycol (PPG 400, PPG 4000) in toluene and aqueous mixture of Polyethelene Glycol (PEG 200) have been estimated for different concentrations (2%, 4%, 6%, 8% & 10%) at 303K and these experimental values are compared with theoretical values obtained by using various mathematical methods like Lorentz-Lorenz equation, Gladstone-Dale equation, Newton's equation, Arago-Biot(AB) equation, Heller equation and Weiner equation. Average Percentage Error (APE) technique is used to match the most accurate method with experimental method. Comparison of evaluated theoretical refractive indices with experimental values reveal the nature of interaction between component molecules in the mixtures.*

Keywords— *Arago Biot, Heller, Lorentz-Lorenz, Polymer, Refractive Index and Weiner.*

I. Introduction

The concept of refractive index "before mixing" is introduced and shown to be given by the volume fraction mixing rule of the pure-component refractive indices. The refractive index of thermodynamically ideal liquid mixtures is given by the volume-fraction mixing rule of the pure-component squared refractive indices[1-6]. Abbe refractometer [7-8] measures the index of refraction by the measurement of the critical angle of total reflection. Polyethylene glycol is used as humectants in inks and adhesives. It acts as a solvent in soldering flux and as a dye carrier in inks. It is also useful as a modifier and binder in latex paint. It is used as an additive in synthetic lubricants, cutting oil and hydraulic fluids. It plays an important role for the precipitation of proteins.

II. Methods and Materials

The polymer solutions are prepared by dissolving PEG 200 in water and PPG 400 and PPG 4000 in toluene to get desired concentrations (2%, 4%, 6%, 8% and 10%). Magnetic stirrer [REMI make] is used for this purpose at a rate of 1000 rpm. Refractive index values are measured using thermostatically controlled Abbe Refractometer having accuracy less than 0.0001 units. Density values are measured using specific gravity method. The mass of the liquid is measured using a K-ROY make electronic balance, with an accuracy of ±0.001gm.

III. Results and Discussion

A. *Evaluation of Theoretical refractive index*

In the present study, refractive index is determined for aqueous mixtures of PEG 200 and PPG 400 and PPG 4000 in toluene at different concentrations (2%, 4%, 6%, 8% & 10%) at 303K temperature. The experimental refractive index values are compared with theoretical refractive indices by Lorentz-Lorenz equation, Gladstone-Dale equation, Newton's equation, Arago-Biot(AB) equation, Heller equation and Weiner equation which are listed below.

The Lorentz-Lorenz (L-L) relation for refractive index is based on the change in the molecular interaction with volume fraction.

$$\left(\frac{n_m^2-1}{n_m^2+2}\right)\frac{1}{\rho_m} = \left(\frac{n_1^2-1}{n_1^2+2}\right)\phi_1 + \left(\frac{n_2^2-1}{n_2^2+2}\right)\phi_2 \qquad (1)$$

where,

$\phi_1 = \frac{w_1}{\rho_1}$ and $\phi_2 = \frac{w_2}{\rho_2}$, w_1 and w_2 are the weight fractions of the pure components 1 and 2 respectively, and ρ_m, ρ_1 and ρ_2 are the density of the mixture, and densities of the pure components 1 and 2 respectively and n_m, n_1 and n_2 are the refractive index of the mixture, refractive indices of the pure components 1and 2 respectively.

The Gladstone–Dale relation is used for optical analysis and also to measure the density of a liquid that is used in fluid dynamics. This relation is also used to calculate refractive index. Gladstone-Dale (G-D) equation for predicting the refractive index of a binary liquid mixture is given below.

$$(n_m - 1) = \phi_1 (n_1 - 1) + \phi_2 (n_2 - 1) \quad (2)$$

where n_m, n_1 and n_2 are the refractive index of the mixture, refractive indices of the pure components 1and 2 respectively.

Weiner's (W) relation can be represented as

$$\left(\frac{n_m^{\,2} - n_1^{\,2}}{n_m^{\,2} + 2n_1^{\,2}}\right) = \left(\frac{n_2^{\,2} - n_1^{\,2}}{n_2^{\,2} + 2n_1^{\,2}}\right)\phi_2 \quad (3)$$

where, $\phi_2 = \frac{w_2}{\rho_2}$, w_2 is the weight fraction of the pure component 2, and ρ_2 is the density of the pure component 2 and n_m, n_1 and n_2 are the refractive index of the mixture, refractive indices of the pure components 1and 2 respectively.

Heller's (H) equation is given by

$$\left(\frac{n_m - n_1}{n_1}\right) = \frac{3}{2}\left(\frac{m^2 - 1}{m^2 + 2}\right)\phi_2 \quad (4)$$

where, $m = \frac{n_2}{n_1}$, $\phi_2 = \frac{w_2}{\rho_2}$, w_2 is the weight fraction of the pure component 2, and ρ_2 is the density of the pure component 2 and n_m, n_1 and n_2 are the refractive index of the mixture, refractive indices of the pure components 1and 2 respectively.

Arago-Biot (A-B), assuming volume additively, proposed the below mentioned relation for refractive index of binary liquid mixtures.

$$n_m = \phi_1 n_1 + \phi_2 n_2 \quad (5)$$

where, $\phi_1 = \frac{w_1}{\rho_1}$ and $\phi_2 = \frac{w_2}{\rho_2}$, w_1 and w_2 are the weight fractions of the pure components 1 and 2 respectively, and ρ_m, ρ_1 and ρ_2 are the density of the mixture, and densities of the pure components 1 and 2 respectively and n_m, n_1 and n_2 are the refractive index of the mixture, refractive indices of the pure components 1 and 2 respectively.

Newton (N) gave the following equation

$$(n_m^{\,2} - 1) = \phi_1 (n_1^{\,2} - 1) + \phi_2 (n_2^{\,2} - 1) \quad (6)$$

where, $\phi_1 = \frac{w_1}{\rho_1}$ and $\phi_2 = \frac{w_2}{\rho_2}$, w_1 and w_2 are the weight fractions of the pure components 1 and 2 respectively, and ρ_m, ρ_1 and ρ_2 are the density of the mixture, and densities of the pure components 1 and 2 respectively and n_m, n_1 and n_2 are the refractive index of the mixture, refractive indices of the pure components 1and 2 respectively.

The percentage of deviation is calculated by the following equation

$$APE = 1/n \sum [(R.I._{\exp} - R.I._{cal}) / R.I._{\exp}] * 100 \quad (7)$$

where n is the number of data used, $R.I._{exp}$ is the experimental refractive index and $R.I._{cal}$ is the theoretical refractive index.

The experimentally measured refractive index and the estimated refractive index from various mathematical models like Lorentz-Lorenz equation, Gladstone-Dale equation, Newton's equation, Arago-Biot (AB) equation, Heller equation and Weiner equation [1-6] for the binary liquid mixture of aqueous solution of PEG 200 & PPG 400 and PPG 4000 in toluene at five different concentrations at 303K are presented in the Table 1. From this table, it is observed that the experimental values of refractive index increases with increase in concentration for aqueous solution of PEG 200 and decrease in concentration for PPG 400 & PPG 4000 in toluene. The average percentage of deviation is estimated for all systems taken for study and the values are listed in Table 2.

IV. Conclusion

For PEG 200, the percentage of deviation is higher in Lorentz-Lorenz relation. Very less variation from experimental method is observed in Arago-Biot relation. Hence, Arago-Biot relation is the most suitable relation for estimating the refractive index of PEG 200 taken for study as the value obtained using this method closely matches with experimental data.

For PPG 400 & PPG 4000, the percentage of deviation is higher in Lorentz-Lorenz relation. Very less variation from experimental method is observed in Gladstone-Dale equation. Hence, Galdstone-Dale equation may be the most reliable model for estimating refractive index in the PPG 400 & 4000 taken for study.

System	Conc.% gm/ml	Expt R. I.	Lorentz-Lorenz	Gladstone-Dale	Arago-Biot	Heller	Newton	Wiener
PEG 200 + Water	2	1.341	1.3418	1.3416	1.3458	1.3383	1.3414	1.3397
	4	1.343	1.3419	1.3418	1.3454	1.3385	1.3416	1.3399
	6	1.346	1.3420	1.3419	1.3457	1.3387	1.3417	1.3401
	8	1.348	1.3942	1.3420	1.3456	1.3389	1.3419	1.3403
	10	1.350	1.3422	1.3422	1.3455	1.3391	1.3420	1.3405
PPG 400 + Toluene	2	1.494	1.4942	1.4939	1.4935	1.4944	1.4944	1.4947
	4	1.493	1.4945	1.4937	1.4945	1.4942	1.4945	1.4944
	6	1.492	1.4947	1.4935	1.4955	1.4940	1.4946	1.4942
	8	1.49	1.6215	1.4933	1.4965	1.4938	1.4947	1.4940
	10	1.489	1.4951	1.4932	1.4975	1.4935	1.4947	1.4938
PPG 4000 + Toluene	2	1.495	1.5940	1.5756	1.7399	1.5013	1.5611	1.5015
	4	1.494	1.5932	1.5746	1.7385	1.5010	1.5605	1.5013
	6	1.493	1.5925	1.5737	1.7370	1.5008	1.5600	1.5010
	8	1.491	1.7532	1.5728	1.7355	1.5005	1.5595	1.5008
	10	1.486	1.5910	1.5719	1.7341	1.5003	1.5589	1.5006

Table 1. Experimental and mathematical refractive index for PEG and PPG

System	Conc(%) gm/ml	Expt. R.I	Lorentz-Lorenz	Gladstone-Dale	Arago-Biot	Heller	Newton	Wiener
PEG 200 + Water	2	1.3410	0.00057	0.00047	0.00361	0.00205	0.00034	0.00098
	4	1.3430	0.00084	0.00093	0.00178	0.00337	0.00105	0.00231
	6	1.3460	0.00299	0.00305	0.00024	0.00543	0.00318	0.00437
	8	1.3475	0.03462	0.00406	0.00141	0.00638	0.00418	0.00532
	10	1.3500	0.00578	0.00580	0.00332	0.00806	0.00593	0.00701
APE			**4.5**	**1.4**	**1.0**	**2.5**	**1.5**	**2.0**
PPG 400 + Toluene	2	1.494	0.00016	0.00005	0.00034	0.00030	0.00026	0.00046
	4	1.493	0.00098	0.00048	0.00102	0.00081	0.00099	0.00097
	6	1.492	0.00181	0.00102	0.00237	0.00133	0.00172	0.00149
	8	1.49	0.08825	0.00224	0.00439	0.00252	0.00312	0.00268
	10	1.489	0.00412	0.00279	0.00573	0.00304	0.00386	0.00320
APE			**9.5**	**0.7**	**1.4**	**0.8**	**1.0**	**0.9**
PPG 4000 + Toluene	2	1.495	0.00051	0.00072	0.00100	0.00037	0.00041	0.00021
	4	1.494	0.00031	0.00019	0.00035	0.00014	0.00032	0.00030
	6	1.493	0.00114	0.00035	0.00170	0.00066	0.00105	0.00082
	8	1.491	0.08752	0.00157	0.00372	0.00185	0.00245	0.00200
	10	1.486	0.00615	0.00482	0.00776	0.00507	0.00588	0.00522
APE			**9.6**	**0.7**	**1.5**	**0.8**	**1.0**	**0.9**

Table 2. Values of Average Percentage Error (APE) for PEG 200, PPG 400 and PPG 4000

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