TuijinJishu/Journal of Propulsion Technology
ISSN: 1001-4055
Vol. 44 No.6 (2023)

Modeling and Correlation of Physical Properties of Ternary Liquid Mixtures

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***Abstract*:**

Densities, viscosities, and refractive indices of a ternary system and three component binary systems at T=298.15 K were determined at atmospheric pressure and across the concentration range. The measured values of density were used to determine the observed values of excess volumes. These results were used to calculate refractive index deviations (Δn), viscosity variances ($\Delta\eta$), and excess molar volumes (V^E). Redlich - Kister polynomials of variable degrees were fitted to the estimated values of V^E, η, and n. The ternary results were compared with the values estimated by a number of theoretical equations of prediction, including the McAllister three- and four-body interaction models, Flory model, Glinski model, and (RS) model. In conclusion, by using V^E, $\Delta\eta$, and Δn, these models can aid in our understanding of the characteristics and interactions pertaining to liquids. When we compared the results of the experiment and theory, we discovered some degree of consistency.

Keywords:*Physical properties, Fluid mixture,Modeling, Correlations*

1. Introduction:

Important fundamental information used in process simulation, equipment design, solution theory, and molecular dynamics includes density, viscosity, and refractive index [1, 2]. A deeper comprehension of viscosity is crucial for constructing computations involving heat transfer, mass transfer, and fluid movement and is of great physico-chemical importance. Viscosity is a concept that is frequently employed in product compositions and processing [3] in many industrial applications. The octane number of gasoline is typically increased by adding a few oxygenated chemicals, which also helps to cut down on pollution. The oxygenated compounds of the type "cyclic ether or aliphatic alcohol" and the alkane liquid that is typically found in gasoline are the subjects of the current paper. Cyclic ethers can be seen as an intermediary instance between alkanes (inert chemicals) and alkanols (highly self-associatedcompounds) from the perspective of association. Due to these factors, we evaluated the densities, viscosities, excess volumes and refractive indices of binary and ternary mixes of 2,2,4-trimethylpentane, tetrahydrofuran, and 2-propanol at atmospheric pressure over the whole concentration range. Previous studies [4–7] have outlined the precise measurement techniques used for these measurements [1-2]. The Lorentz-Lorentz (L-L) connection [8-9], the Flory model [10-12], the Glinski model [13], and the Ramaswamy and Anbananthan (RS) model [14] were all used to investigate these data. While the Flory model (non-associated) is based on the additivity of liquids, the RS and Glinski model (associated) are based on the association constant as an adjustable parameter. These findings led to the determination of the binary coefficients and standard errors, which were then calculated and fitted to the Redlich-

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Kister type polynomial equation [15]. Additionally, an effort has been made to correlate the experimental results with the McAllister equation [16].

2. Experimental Section:

2.1*Materials*

Solvent materials of high purity and AR grade were purchased from Merck Co. for use in this investigation Inc., Germany, and utilized unpurified. To reduce the amount of water in the liquids, they were placed in opaque bottles over 0.4 nm molecular sieves. Gas chromatography was used to determine the purity of each chemical, and the findings showed that the mass purity was greater than 0.95. Without additional purification, all of the components were utilized. At T = 298.15 K, the densities, viscosities, and refractive indices of these components nearly matched the values reported in the approved literature [17–19] (Table 1).

2.2 *Apparatus and Procedure*

We calibrated the equipment using doubly distilled water at atmospheric pressure before to each series of trials. The published values were within $1 \cdot 10^{-3}$kg.m^{-3} of the expected density measurement error. Using a bi-capillary pyknometer, the densities of the pure components and their mixes were measured. Using an electronic balance model Shimadzuax-200 that is accurate to within 0.1 mg, the liquid combinations were made by mass in an airtight stopper bottle. The mixtures' average compositional uncertainty was calculated to be less than 0.0001 on average. The IUPAC relative atomic mass table served as the foundation for all molar amounts.

Using a Canon Ubbelohde suspended-level viscometer, the viscosities of pure liquids and mixes were determined at atmospheric pressure and at various temperatures. The temperature of the water bath (Raga Industries) in which the viscometer was submerged was controlled to within 0.01 K. A digital stopwatch with a precision of 0.01s was used to record the flow time. Results were averaged after each experiment was run four times at each temperature for all compositions. The liquid's viscosity was then determined using the following relationship;

$$v = \eta / \rho = k (t - \theta)$$

(1)(1)Where v is the kinematic viscosity, η, is the dynamic viscosity, ρ, is the density, t is the flow duration, k and $\theta$are the viscometer constant, and is the Hagen Bach correction factor. Viscosity measurements were said to have an estimated uncertainty of less than 0.001 m Pa.s. and reproducibility of less than $6 \cdot 10^{-3}$ m Pa.s. An Atago -3T Abbe refractometer with thermostatic control was used to test refractive indices. The accuracy of the measurements of the refractive index was 0. 0001.Thedetailedmeasuringproceduresforthese measurements have been described in previous studies [4-7].The uncertainty in the ρ, η, and $n$wasestimatedtobe$1 \cdot 10^{-3}$g·cm^{-3},0.006 mPa·s, $2 \cdot 10^{-4}$,respectively.

3. Modeling:

Based on the hypothesis that thermodynamic and physico-chemical properties of ternary liquid mixtures can be inferred from their contributing binaries, Bertrand, Acree, and colleagues [20–23] have constructed a prediction equation. The general mixing equation is obeyed by this equation because,

$$\Delta Z_{123}^{-ex} = (n_1\Gamma_1 + n_2\Gamma_2 + n_3\Gamma_3)^{-1}(n_1\Gamma_1 n_2\Gamma_2 A_{12} + n_1\Gamma_1 n_3\Gamma_3 A_{13} + n_2\Gamma_2 n_3\Gamma_3 A_{23}) \qquad (2)$$

Z_{123} stands for any significant thermodynamic feature that can be expressed in terms of the interaction parameters A_{ij} and the weighting factors *i*. This equation produces a fairly accurate predictive form when the characteristics of binary systems are combined.

Review of the equation(2) reveal that for systems obeying this equation, the properties of the contributing binary systems would obey (per mole of ternary solution) the following equation:

$$\Delta Z_{ij}^{-ex} = X_i^* X_j^* \Gamma_i \Gamma_j A_{ij} / (X_i^* \Gamma_i + X_j^* \Gamma_j) \quad (3)$$

For one mole of ternary solution, eq. (2) can be rearranged to,

$$\Delta Z_{123}^{-ex} = (X_1 + X_2)(f_1 + f_2)(\Delta Z_{12}^{-ex})^* + (X_1 + X_3)$$
$$(f_1 + f_3)(\Delta Z_{13}^{-ex})^* + (X_2 + X_3)(f_2 + f_3)(\Delta Z_{23}^{-ex})^* \quad (3)$$

In general for the multi-component system, eq. (2) can be rearranged to,

$$\Delta Z_{12....N}^{-ex} = \sum_{i=1} \sum_{j>1}^{N} (X_i + X_j)(f_i + f_j)(\Delta Z_{ij}^{-ex})^* \quad (4)$$

However, Bertrand et al. [23] have provided a method for calculating the ratio of raw weighting components. The multi-component system's components are merged to normalize the weighting factors to an average value of 100, where ratio is calculated for each binary combination.

$$\Gamma_i = (100N)[(\Gamma_1^{raw} / \Gamma_i^{raw}) + (\Gamma_2^{raw} / \Gamma_i^{raw}) + ...$$
$$+ (\Gamma_N^{raw} / \Gamma_i^{raw})] \quad (5)$$

Excess physical attributes can be obtained in light of the aforementioned equations, where eq. (4) has the following form:

$$\Delta Z_{123}^{E} = \sum_{i=1}^{3} \sum_{j>1}^{3} (X_i + X_j)(\phi_i + \phi_j)(\Delta Z_{ij}^{E}) \quad (6)$$

3.1 *Ramaswami and Anbananthan Model*

The model was put up by Ramswamy and Anbananthan [14] and is predicated on the notion that acoustic impedance is linear with respect to component mole fraction. Here, it is assumed that any linearly dependent physical property, like viscosity, refractive index, surface tension, etc., may be predicted [21–25]. Glinski [13] also made the following additional assumptions regarding how molecules interact when a solute is given to a solvent:

$$A+B = AB \quad (7)$$

and the association constant K_{as} can be defined as;

$$K_{as} = \frac{[AB]}{[A][B]} \quad (8)$$

Where*A* is the solvent concentration and *B* is the solute concentration in the liquid combination. Applying the linearity with composition requirement

$$Z_{obs} = x_A Z_A + x_{AB} Z_{AB} \quad (9)$$

Where, respectively, x_A, x_{AB}, Z_A, Z_{AB}, and Z_{obs} represent the mole fractions of *A*, associate *AB*, and the physical characteristics (viscosity and refractive index) of *A*, associate *AB*, and the observed physical characteristics. It is impossible to acquire the component *AB* in its purest form. Here, the equilibrium response is by definition incomplete because the mixtures also contain molecules from unrelated components. Thus, the eq. (9) assumes the shape of;

$$Z_{obs} = [x_A Z_A + x_B Z_B + x_{AB} Z_{AB}] \quad (10)$$

However, I was able to use and detail out the main notion of this approach in my earlier work [4-7].

3.2 *Corrected model of Ramaswami and Anbanthan*

Glisnki offered the equation assuming additivity with the volume fraction, of the components derived by Natta and Baccardedda [24] after reviewing the Ramaswamy and Anbananthan model's results.

$$Z_{cal} = \frac{Z_1 Z_2}{\phi_1 Z_2 + \phi_2 Z_1}$$

(11)Where 1, 2 are the volume fractions of components 1 and 2, Z_1 and Z_2 are the physical characteristics of the individual pure component liquids, and Z_{cal} is the theoretical physical qualities of the binary liquid mixture.

3.3 *Flory Model*

According to Macedo and Litovitz's [25] combination of the absolute rate theory and free volume theory provides of the probability for obtaining adequate activation energy and the occurrence of an empty site.`Roseveane et al. [26] interconnected the thermodynamic functions of mixing by assuming a simple relationship between free energy of activation $\Delta G^{\neq}$, and the residual Gibbs free energy of mixing ΔG_M^R. as;

$$\Delta G^{\neq} = \sum_{i=1}^{2} x_i \Delta G_i^{\neq} - \alpha \Delta G_M^R$$

(12)Where $\Delta G_M{}^R$ the residual free energy of is mixing, α is a constant of order unity and $\Delta G_i{}^{\neq}$ is the activation free energy of ith component liquid. When we increase the residual free energy of mixing contributions and use the value of activation energy as a replacement, we obtain,

$$\ln\eta = \sum_{i=1}^{2} x_i \ln\eta_i - \Delta G_M^R / RT + v^* \{(1-v_f) - (\sum_{i=1}^{2} x_i / V_{f_i})\}$$

(13)The value of $\Delta G_M{}^R$ for binary liquid mixture can be evaluated as detailed out by Flory [6-8] as;

$$\Delta G_M^R = x_1 P_1^* V_1^* \left[\left(\frac{1}{\tilde{V}_1} - \frac{1}{\tilde{V}} \right) + 3\tilde{T}_1 \ln \frac{(\tilde{V}_1^{1/3} - 1)}{(\tilde{V}^{1/3} - 1)} \right]$$

$$+ x_2 P_2^* V_2^* \left[\left(\frac{1}{\tilde{V}_2} - \frac{1}{\tilde{V}} \right) + 3\tilde{T}_2 \ln \frac{(\tilde{V}_2^{1/3} - 1)}{(\tilde{V}^{1/3} - 1)} \right] + \frac{x_1 P_1^* V_1^* \theta_2 X_{12}}{\tilde{V}_1}$$

(14)By substituting the value of $\Delta G_M{}^R$ in eq (12), we obtain the final expression for the dynamic viscosity of binary liquid mixture as;

$$\ln\eta = x_1 \ln\eta_i + x_2 \ln\eta_2 - [x_1 P_1^* v_1^* \{(1/\tilde{v}_1 - 1/\tilde{v}_1) +$$

$$3\tilde{T}_1 \ln\{(\tilde{v}_1^{1/3} - 1)/(\tilde{v}^{1/3} - 1)\} + x_2 P_2 v_2^* \{(1/\tilde{v}_2 - 1/\tilde{v}) + 3\tilde{T}_2$$

$$\ln\{(\tilde{v}_2^{1/3} - 1)/(\tilde{v}^{1/3} - 1)\} + x_1 v_1^* \theta_2 X_{12} / \tilde{v}_1] / RT + 1/\{(\tilde{v} - 1) - x_1/(\tilde{v}_1 - 1) - x_2/(\tilde{v}_2 - 1)$$

(15)The equation for excess molar volume according to Flory theory can be expressed as

$$\tilde{V} - \tilde{V}_0 = V^E = \frac{V^E}{x_1 V_1^* + x_2 V_2^*} \qquad (16)$$

The ideal reduced volume ($\tilde{V}_0$) is related to

$$\tilde{V}_0 = \psi_1 V_1 + \psi_2 \tilde{V}_2 \qquad \text{and} \qquad (17)$$

$$V^E = (x_1 V_1^* + x_2 V_2^*)[\tilde{V} - (\psi_1 \tilde{V}_1 + \psi_2 \tilde{V}_2)] \qquad (18)$$

The method described by Flory [10–12] and others [5, 27] is used to determine the values of the reduced and characteristic parameters by the equation as detailed out earlier [5], and the notations used have their customary significance.

The viscosity of liquid mixtures and mole fraction are frequently correlated using the McAllister multi-body interaction model [16]. A definition of the three-body model is detailed out earlier [4-7].

3.4 *Lorentz-Lorentz Relation*

The Lorentz-Lorentz (L-L) relation [8–9] is widely used in evaluating mixture refractive indices, pure component densities, and mixture density. It is represented in terms of specific refraction as follows:

$$\left[\frac{n^2-1}{n^2+2}\right]\frac{1}{\rho}=\left[\frac{n_1^2-1}{n_1^2+2}\right]\frac{w_1}{\rho_1}+\left[\frac{n_2^2-1}{n_2^2+2}\right]\frac{w_2}{\rho_2} \qquad (19)$$

Another use of this relationship, where is taken into account

$$\left[\frac{n^2-1}{n^2+2}\right]=\left[\frac{n_1^2-1}{n_1^2+2}\right]\phi_1+\left[\frac{n_2^2-1}{n_2^2+2}\right]\phi_2 \qquad (20)$$

Here, *n*, n_1, n_2, $\varphi_1\varphi_2$, w_1, w_2, density of mixture, density of pure components, weight fraction of pure components, and 1, 2 are the volume fractions of pure components, which are given by the relation [28] as: $\phi_i=\frac{x_i v_i}{\sum x_i v_i}$ (21)

Wherex_i, v_i are the mole fraction and molar volume of the ith component.

4.Results and Discussion:

We [5-7] and others [29] have already extensively tested the values of *α*and β_T derived from such an expression.

$$\beta_T=\frac{1.71\times10^{-3}}{T^{4/9}u^2\rho^{4/3}} \quad \text{and} \quad \alpha=\frac{75.6\times10^{-3}}{T^{1/9}u^{1/2}\rho^{1/3}} \qquad (22)$$

The Redlich-Kister equation [12] was used to mathematically express the mixing function,$\Delta\eta$ &Δ *n*, and to correlate the experimental data as follows:

$$y=x_i(1-x_1)\sum_{i=0}^{p}a_i(2x_1-1)^i \qquad (23)$$

Where x_i is the mole fraction and a_i is the coefficients, *y* denotes $\Delta\eta$ &Δ *n*. The standard deviations between the experimental and fitted values of each function, as well as the coefficients a_i values, are listed in Table 2 as a result of a multiple regression analysis using the least squares approach. The definition of the standard deviation is.

$$\sigma=\left[\sum_{i=1}^{m}(y_{\exp_i}-y_{cal_i})^2/(m-p)\right]^{1/2} \qquad (24)$$

Where*p* is the number of movable parameters and m is the number of experimental points. In terms of viscosity, the values range from 0.03 to 3.5 m Pa.s, with the largest value corresponding to a mixture of tetrahydrofuran (1) and 2-propanol (2) at 298.15 K. In terms of refractive index, the values range from 0.08 to 0.016, with the largest value corresponding to the same mixture at 298.15 K.Table 3 provides the estimated viscosity equation parameters and the standard deviations, between the calculated and observed values.

Table 1.PropertiesofthePureLiquids.

Components	***T/K***	***ρ/ $g{\cdot}cm^{-3}$***		***η/mPa.s***		***n***	
		exp	***lit***	***exp***	***lit***	***exp***	***lit***
tetrahydrofuran	298.15	0.8821	0.8829	0.474	0.530	1.4058	1.4049
2-propanol	298.15	0.7817	0.78126	2.074	2.0436	1.3761	1.3752
2,2,4-trimethylpentane	298.15	0.6882	0.68781	0.486	0.4802	1.3901	1.38898

Table 2.Parameters of Redlich-KisterandStandardDeviation(δ)forBinaryMixture.

ΔQ_{ij}	***T/K***	a_0	a_1	a_2	a_3	$\delta{\cdot}10^3$
Tetrahydrofuran(1)+ 2-Propanol(2)						
V^E/cm^3·mol^{-1}	298.15	0.7557	0.1702	0.0648	−0.0077	1.2
$\Delta\eta$/mPa·s	298.15	−2.3937	1.5864	−0.9552	0.4843	3.5
Δn	298.15	−0.00143	0.0011	0.0016	−0.0004	0.016
Tetrahydrofuran(1)+2,2,4-Trimethylpentane(3)						
V^E/cm^3·mol^{-1}	298.15	0.4776	−0.5698	0.1764	0.3040	1.9
$\Delta\eta$/mPa·s	298.15	−0.017	0.0097	−0.0002	−0.0215	0.03
Δn	298.15	-0.01119	−0.0017	0.0016	-3.28×10^{-6}	0.012
2-Propanol(2)+2,2,4-Trimethylpentane(3)						
V^E/cm^3·mol^{-1}	298.15	2.1573	−0.9151	0.1620	0.2617	2.8
$\Delta\eta$/mPa·s	298.15	−2.4628	−1.3894	−0.7292	−0.7782	2.4
Δn	298.15	0.0045	0.0039	−0.0021	0.0014	0.08

Table3.Parameters of Redlich-KisterandStandardDeviation(δ)for TernaryMixture.

Tetrahydrofuran (1) + 2-Propanol (2) + 2,2,4-Trimethylpentane (3)

ΔQ123	***C00***	***C10***	***C01***	***C11***	***C20***	***C02***	***δ · 103***
V^E/cm^3 · mol^{-1}	2.123	-14.050	-6.596	16.332	18.265	10.260	10.5
$\Delta\eta$/mPa · s	9.649	-57.105	20.372	3.974	-4.599		6.5
Δn	-0.401	1.105	1.173	-1.293	-1.036	-1.162	0.61

It was shown that the four body model of the McAllister equation greatly outperformed the three body model in its ability to accurately correlate the mixture viscosity for all of the systems. In addition, a declining trend in the values of the McAllister parameters has been seen with the decrease of composition.In most cases, McAllister's models are sufficient for

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correlating systems with minor variations. These equations have also been effectively applied to refractive index prediction.The success of all the theoretical models is demonstrated by the theoretical findings, which are quite close to the experimental data. Through the fitted viscosity and refractive index values in a fictitious pure associate and observed dependence of concentration on composition of a mixture, the associated processes model developed by Ramaswamy and Anbananthan provides more reliable results and is useful in determining the internal structure of associates. The outcomes may certainly be improved, though. In order to interpret the associational behaviour and interactions in liquid mixtures, several changes are still generally required.

Tables 4 through 7 provide the experimental results of, η,n for binary mixes and ternary mixtures of tetrahydrofuran, 2-propanol, and 2,2,4-trimethylpentane at T=298.15 K. The valuesof, η, and n for each of these binary systems drop as the composition increases. The trend of variation of dynamic viscosity with compositions in all the binary systems are uniform and in identical manner as shown in tables 4and 5. The values of the molar excess volumes (V^E), viscosity deviations ($\Delta\eta$), and refractive index deviations (Δn) for these binary and ternary mixes at T=298.15 K are shown in tables. The following equation was used to compute the molar excess volumes, or V^E, using density data.

$$v^E = \sum_{i=1}^{N} x_i \boldsymbol{M}_i \left(1/\rho - 1/\rho_i \right) \qquad (25)$$

where the pure component i's mole fraction, molar mass, and density are represented by x_i, M_i, and ρ_I respectively. N is the number of components. Table 4 show that the V^E values are positive for all compositions. Less than 3 • 10^{-3} cm^3 • mol^{-1} of excess molar volume uncertainty was calculated. The values of V^E range from 0.011 cm3 mol-1 to 0.562 cm^3 mol^{-1}. Tetrahydrofuran + 2, 2, 4-trimethylpentane, tetrahydrofuran + 2-propanol, 2-propanol + 2, 2, 4-trimethylpentane raises the excess molar volume [(V^E (x)=0.5)] in that order. The values of V^E for every single one of these binary systems increase up to maximum then decrease as the composition rises. The balance between positive contributions (hydrogen bond rupture or dispersive interactions between dissimilar molecules) and negative contributions can be used to describe how V^E depends on composition for the current mixtures (intermolecular dipolar interactions or geometrical fitting between components). Tetrahydrofuran and 2, 2, 4-trimethylpentane mixtures are related in the current study by a dipole-dipole interaction, while 2-propanol is associated through the hydrogen bonding of its hydroxyl group. The observed V^E in our systems are positive, and the main source of the positive V^E is probably the breakdown of these two types of contacts during mixing. We conclude that the breaking of the H-bond between 2-propanol molecules contributes more to the V^E values than the O-O interaction between tetrahydrofuran molecules since the V^E values in mixes of 2,2,4-trimethylpentane with 2-propanol are higher than those in mixtures with tetrahydrofuran.

$$\Delta z = z - \sum_{i=1}^{N} \dot{x}_i z_i \qquad (26)$$

where the pure liquid i and the physical characteristics of the combination, respectively, are denoted by z and z_i.The binary values over the whole mole fractions are seen to be negative. The values of x_i and x_j for minuscule. The findings of a least-squares method used to calculate the binary interaction coefficients, a_k, are shown in Table 2.

Table 4.Densities (ρ),Viscosities (η) and Theoretical viscosity computed from two different models fortheTetrahydrofuran(1)+2-Propanol(2) +2, 2, 4-Trimethylpentane(3) Ternary Systemat298.15**K.**

x_1	x_2	$\rho/g{\cdot}cm^{-3}$	$\eta_{exp}/mPa{\cdot}s$	$\eta_{Flory}/mPa{\cdot}s$	$\eta_{BAB}/mPa.s$	$\Delta\eta/mPa{\cdot}s$	n_{exp}	n_{BAB}	$n_{L\text{-}L}$	$V^E/cm^3{\cdot}mol^{-1}$	$V^E_{Flory}/cm.^3{\cdot}mol^{-1}$	$\Delta n.10^3$
0.0500	0.9000	0.7758	1.467	1.554	1.546	-0.419	1.3764	1.3784	1.3765	0.104	0.134	–0.89
0.0500	0.7999	0.7580	1.122	1.226	1.206	-0.608	1.3780	1.3799	1.3783	0.242	0.272	–0.70
0.0500	0.7000	0.7436	1.905	2.056	1.996	-0.669	1.3795	1.3814	1.3791	0.382	0.399	–0.63
0.0500	0.6000	0.7318	0.759	0.812	0.817	-0.658	1.3808	1.3827	1.3805	0.477	0.497	–0.69
0.0500	0.5001	0.7220	0.655	0.715	0.723	-0.606	1.3820	1.3841	1.3822	0.531	0.561	–0.86
0.0500	0.4000	0.7138	0.586	0.632	0.641	-0.519	1.3832	1.3853	1.3835	0.567	0.587	–1.10
0.0500	0.3000	0.7069	0.541	0.601	0.611	-0.407	1.3843	1.3863	1.3841	0.545	0.566	–1.38
0.0500	0.2000	0.7011	0.509	0.594	0.603	-0.283	1.3855	1.3874	1.3857	0.474	0.497	–1.63
0.0500	0.1000	0.6965	0.491	0.563	0.571	-0.144	1.3866	1.3883	1.3871	0.304	0.347	–1.88
0.0500	0.0500	0.6944	0.484	0.556	0.563	-0.073	1.3872	1.3891	1.3877	0.210	0.252	–1.97
0.1000	0.8500	0.7806	1.256	1.304	1.326	-0.552	1.3744	1.3763	1.3749	0.131	0.153	–4.37
0.1000	0.7500	0.7623	0.998	1.074	1.001	-0.653	1.3790	1.3812	1.3797	0.290	0.314	–1.15
0.1000	0.6500	0.7477	0.821	0.897	0.913	-0.674	1.3805	1.3824	1.3816	0.387	0.397	–1.08
0.1000	0.5500	0.7358	0.701	0.789	0.811	-0.638	1.3818	1.3837	1.3823	0.462	0.493	–1.16
0.1000	0.4500	0.7258	0.622	0.692	0.707	-0.560	1.3830	1.3849	1.3837	0.512	0.587	–1.35
0.1000	0.3499	0.7174	0.561	0.599	0.623	-0.465	1.3842	1.3863	1.3849	0.526	0.557	–1.60
0.1000	0.2500	0.7103	0.523	0.577	0.578	-0.347	1.3853	1.3872	1.3857	0.500	0.533	–1.89
0.1000	0.1501	0.7045	0.499	0.541	0.551	-0.214	1.3864	1.3883	1.3871	0.399	0.421	–2.14
0.1000	0.0500	0.6997	0.483	0.502	0.523	-0.074	1.3877	1.3897	1.3881	0.214	0.233	–2.33

0.2000	0.7500	0.7901	0.991	1.107	1.099	-0.659	1.3802	1.3819	1.3814	0.186	0.198	–1.51
0.2000	0.6500	0.7712	0.814	0.887	0.909	-0.680	1.3817	1.3837	1.3821	0.314	0.337	–1.47
0.2000	0.5500	0.7561	0.698	0.752	0.797	-0.640	1.3830	1.3849	1.3835	0.391	0.412	–1.58
0.2000	0.4500	0.7437	0.617	0.678	0.683	-0.564	1.3842	1.3861	1.3847	0.436	0.457	–1.78
0.2000	0.3500	0.7334	0.562	0.603	0.634	-0.463	1.3853	1.3871	1.3857	0.450	0.469	–2.05
0.2000	0.2500	0.7246	0.523	0.597	0.613	-0.346	1.3864	1.3883	1.3866	0.446	0.489	–2.34
0.2000	0.1501	0.7174	0.498	0.567	0.578	-0.214	1.3875	1.3894	1.3879	0.363	0.387	–2.64
0.2000	0.0500	0.7112	0.482	0.532	0.567	-0.074	1.3887	1.3907	1.3889	0.235	0.247	–2.88
0.3000	0.6500	0.7995	0.814	0.913	0.903	-0.679	1.3829	1.3851	1.3833	0.237	0.251	–1.81
0.3000	0.5500	0.7801	0.699	0.734	0.754	-0.638	1.3842	1.3863	1.3844	0.324	0.343	–1.93
0.3000	0.4500	0.7645	0.621	0.788	0.799	-0.559	1.3854	1.3873	1.3857	0.381	0.398	–2.15
0.3000	0.3500	0.7516	0.565	0.599	0.612	-0.459	1.3865	1.3884	1.3867	0.400	0.421	–2.47
0.3000	0.2500	0.74092	0.526	0.589	0.609	-0.342	1.3876	1.3897	1.3879	0.390	0.411	–2.72
0.3000	0.1500	0.7320	0.508	0.537	0.551	-0.203	1.3887	1.3899	1.3889	0.322	0.349	–3.06
0.3000	0.0500	0.7243	0.488	0.541	0.567	-0.067	1.3898	1.3912	1.3905	0.241	0.256	–3.34
0.4000	0.5500	0.8091	0.704	0.764	0.784	-0.632	1.3857	1.3877	1.3861	0.256	0.264	–2.02
0.4000	0.4500	0.7891	0.621	0.672	0.679	-0.558	1.3868	1.3889	1.3871	0.320	0.337	–2.28
0.4000	0.3500	0.7729	0.565	0.601	0.632	-0.458	1.3879	1.3898	1.3883	0.353	0.348	–2.59
0.3999	0.2501	0.7596	0.533	0.593	0.619	-0.334	1.3890	1.3911	1.3893	0.346	0.364	–2.93
0.4000	0.1500	0.7484	0.499	0.553	0.573	-0.211	1.3900	1.3914	1.3907	0.317	0.331	–3.33
0.4000	0.0500	0.7393	0.482	0.522	0.532	-0.072	1.3910	1.3929	1.3917	0.208	0.227	–3.65

0.5000	0.4500	0.8187	0.623	0.632	0.648	-0.556	1.3885	1.3902	1.3888	0.265	0.287	–2.14
0.5000	0.3500	0.7981	0.566	0.607	0.637	-0.456	1.3895	1.3916	1.3897	0.309	0.323	–2.56
0.5000	0.2500	0.7814	0.531	0.578	0.589	-0.335	1.3905	1.3924	1.3913	0.304	0.3017	–2.99
0.5000	0.1501	0.7677	0.501	0.556	0.565	-0.208	1.3914	1.3933	1.3923	0.271	0.297	–3.43
0.5000	0.0500	0.7564	0.482	0.522	0.547	-0.071	1.3925	1.3944	1.3927	0.173	0.197	–3.77
0.6000	0.3500	0.8284	0.570	0.599	0.617	-0.451	1.3916	1.3935	1.3925	0.247	0.269	–2.00
0.6000	0.2500	0.8077	0.527	0.579	0.603	–0.338	1.3925	1.3941	1.3929	0.255	0.266	–2.53
0.6000	0.1500	0.7901	0.498	0.543	0.565	–0.211	1.3934	1.3955	1.3937	0.225	0.273	–3.05
0.6000	0.0500	0.7761	0.479	0.521	0.561	–0.073	1.3943	1.3962	1.3947	0.140	0.167	–3.50
0.7000	0.2500	0.8385	0.528	0.545	0.547	–0.336	1.3946	1.3967	1.3952	0.190	0.217	–2.03
0.7000	0.1500	0.8165	0.499	0.543	0.557	–0.209	1.3953	1.3971	1.3957	0.196	0.223	–2.69
0.6999	0.0500	0.7990	0.481	0.522	0.543	–0.070	1.3962	1.3983	1.3966	0.118	0.129	–3.24
0.8000	0.1500	0.8484	0.503	0.537	0.541	–0.204	1.3976	1.3995	1.3979	0.136	0.151	–2.03
0.8000	0.0500	0.8260	0.482	0.531	0.537	–0.068	1.39915	1.4009	1.3993	0.090	0.119	–1.88
0.8999	0.0501	0.8585	0.481	0.517	0.522	–0.068	1.40186	1.4027	1.4009	0.052	0.096	–0.74

Table5.Densities (ρ),Viscosities (η) and Theoretical viscosity computed from different models fortheTetrahydrofuran(1)+2-Propanol(2)System at 298.15K

x_1	ρ/ g·cm^{-3}	η_{exp}/ mPa·s	η_{Flory}/ mPa.s	η_{RS}/ mPa.s	$\eta_{Glinski}$/ mPa.s	η_{McA3}/ mPa.s	η_{McA4y}/ mPa.s	n_{exp}	n_{L-L}	n_{RS}	$n_{Glinski}$	n_{McA3}	n_{McA4}
0.0000	0.7811	2.043	1.732	2.262	2.211	2.1022	2.093	1.3751	1.3767	1.3733	1.3767	1.3755	1.3746
0.0500	0.7863	1.706	1.536	1.987	1.932	1.823	1.922	1.3766	1.377	1.3759	1.3774	1.3767	1.3752
0.1000	0.7913	1.445	1.301	1.664	1.721	1.408	1.454	1.3780	1.3789	1.3771	1.3785	1.3785	1.3778

0.1500	0.7963	1.248	1.112	1.446	1.554	1.511	1.1.361	1.3794	1.3796	1.3784	1.3795	1.3797	1.3791
0.2001	0.8013	1.113	1.001	1.267	12.240	1.1.102	1.1.096	1.3808	1.3817	1.3797	1.3814	1.3813	1.3799
0.2500	0.8063	0.988	0.911	1.109	1.164	0.0.997	0.999	1.3823	1.3836	1.3811	1.3833	1.3827	1.3821
0.3000	0.8113	0.896	0.872	0.987	0.997	0.0.963	0.947	1.3837	1.3846	1.3823	1.3845	1.3842	1.3829
0.3500	0.8163	0.812	0.727	0.969	0.972	0.0.889	0.907	1.3851	1.3869	1.3831	1.3864	1.3855	1.3842
0.4000	0.8213	0.752	0.716	0.874	0.901	0.0.814	0.896	1.3866	1.3871	1.3841	1.3874	1.3874	1.3861
0.4500	0.8263	0.703	0.691	0.801	0.879	0.0.773	0.812	1.3881	1.3888	1.3859	1.3888	1.3887	1.3875
0.5000	0.8312	0.659	0.617	0.751	0.788	0.0.712	0.747	1.3896	1.3899	1.3888	1.3899	1.3899	1.3891
0.5500	0.8363	0.623	0.601	0.701	0.735	0.0.686	0.701	1.3911	1.3921	1.3897	1.3921	1.3917	1.3907
0.6000	0.8413	0.594	0.589	0.624	0.669	0.0.644	0.669	1.3926	1.3931	1.3917	1.3938	1.3931	1.3917
0.6500	0.8463	0.567	0.522	0.595	0.617	0.0.611	0.621	1.3942	1.3947	1.3939	1.3951	1.3961	1.3933
0.7000	0.8514	0.545	0.507	0.521	0.578	0.0.576	0.606	1.3957	1.3968	1.3951	1.3966	1.3966	1.3954
0.7500	0.8565	0.526	0.498	0.527	0.521	0.0.542	0.589	1.3973	1.3981	1.3963	1.3983	1.3977	1.3966
0.8000	0.8616	0.511	0.488	0.517	0.503	0.0.511	0.563	1.3988	1.3994	1.3974	1.3994	1.3987	1.3981
0.8500	0.8668	0.497	0.473	0.502	0.498	0.0.497	0.511	1.4004	1.4011	1.3996	1.4014	1.3999	1.3997
0.9000	0.8720	0.488	0.461	0.496	0.474	0.0.491	0.479	1.4019	1.4031	1.4005	1.4023	1.4021	1.4023
0.9500	0.8772	0.480	0.437	0.493	0.463	0.0.48	0.463	1.4033	1.4047	1.4021	1.4041	1.4037	1.4024

						8							
1.0000	0.8823	0.470	0.422	0.482	0.459	0. 0.423	0.454	1.4048	1.4056	1.4033	1.4067	1.4053	1.4036

Table 6.Densities (ρ),Viscosities (η) and Theoretical viscosity computed from different models fortheTetrahydrofuran(1)+2, 2, 4-Trimethyl-pentane(3) at 298.15K

x_1	ρ/ g·cm^{-3}	η_{exp}/ mPa·s	η_{Flory}/ mPa.s	η_{RS}/ mPa.s	$\eta_{Glinski}$/ mPa.s	η_{McA3}/ mPa.s	η_{McA4y}/ mPa.s	n_{exp}	n_{L-L}	n_{RS}	$n_{Glinski}$	n_{McA3}	n_{McA4}
0.0000	0.6879	0.481	0.503	0.592	0.603	0.503	0.536	1.3891	1.3894	1.3887	1.3894	1.3893	1.3889
0.1000	0.6977	0.479	0.499	0.587	0.598	0.501	0.531	1.3898	1.3899	1.3893	1.3899	1.3899	1.3892
0.2000	0.7086	0.477	0.489	0.583	0.579	0.497	0.529	1.3907	1.3903	1.3903	1.3909	1.3903	1.3901
0.3000	0.7210	0.475	0.487	0.578	0.569	0.484	0.524	1.3916	1.3922	1.3911	1.3923	1.3919	1.3911
0.4000	0.7351	0.474	0.469	0.567	0.562	0.481	0.517	1.3928	1.3937	1.3921	1.3931	1.3931	1.3927
0.5000	0.7513	0.473	0.467	0.563	0.556	0.478	0.513	1.3942	1.3951	1.3937	1.3945	1.3947	1.3937
0.6000	0.7699	0.472	0.468	0.546	0.563	0.471	0.511	1.3958	1.3966	1.3951	1.3961	1.3962	1.3952
0.7000	0.7914	0.472	0.451	0.537	0.555	0.469	0. 507	1.3977	1.3978	1.3971	1.3981	1.3981	1.3972
0.8000	0.8165	0.471	0.436	0.533	0.549	0.482	0.501	1.3999	1.3997	1.3991	1.3997	1.3999	1.3991
0.9000	0.8463	0.471	0.427	0.523	0.547	0.467	0.498	1.4022	1.4027	1.4001	1.4020	1.4027	1.4000
1.0000	0.8823	0.470	0.423	0.519	0.533	0.465	0.488	1.4048	1.4051	1.4041	1.4052	1.4053	1.4043

Table 7.Densities (ρ),Viscosities (η) and Theoretical viscosity computed from different models forthe2-Propanol(2)+2, 2, 4-Trimethylpentane(3) System at 298.15K

x_1	ρ/ g·cm^{-3}	η_{exp}/ mPa·s	η_{Flory}/ mPa.s	η_{RS}/ mPa.s	$\eta_{Glinski}$/ mPa.s	η_{McA3}/ mPa.s	η_{McA4y}/ mPa.s	n_{exp}	n_{L-L}	n_{RS}	$n_{Glinski}$	n_{McA3}	n_{McA4}
298.15K													
0.0000	0.6879	0.481	0.535	0.541	0.555	0.497	0.505	1.3891	1.3897	1.3895	1.3895	1.3893	1.3886

0.1000	0.6977	0.479	0.533	0.543	0.553	0.495	0.501	1.3877	1.3889	1.3879	1.3879	1.3881	1.3873
0.2000	0.7086	0.477	0.531	0.539	0.551	0.496	0.499	1.3865	1.3869	1.3869	1.3869	1.3869	1.3862
0.3000	0.7210	0.475	0.529	0.537	0.549	0.493	0.497	1.3854	1.3861	1.3859	1.3856	1.3859	1.3852
0.4000	0.7351	0.474	0.527	0.538	0.548	0.491	0.495	1.3842	1.3855	1.3853	1.3844	1.3843	1.3839
0.5000	0.7513	0.473	0.524	0.535	0.545	0.487	0.493	1.3830	1.3841	1.3837	1.3834	1.3833	1.3827
0.6000	0.7699	0.472	0.522	0.533	0.543	0.483	0.491	1.3817	1.3823	1.3823	1.3821	1.3823	1.3815
0.7000	0.7914	0.472	0.519	0.536	0.541	0.481	0.489	1.3803	1.3811	1.3801	1.3809	1.3806	1.3801
0.8000	0.8165	0.471	0.517	0.534	0.544	0.483	0.486	1.3787	1.3793	1.3779	1.3791	1.3791	1.3785
0.9000	0.8463	0.471	0.518	0.532	0.541	0.479	0.483	1.3770	1.3778	1.3763	1.3776	1.3773	1.3767
1.0000	0.8823	0.470	0.515	0.531	0.539	0.477	0.481	1.3751	1.3763	1.3755	1.3766	1.3755	1.3749

Most of the compositions have negative *n* values. The *n* values are negative for binary mixes of tetrahydrofuran and 2-propanol, while some positive values have been observed at large tetrahydrofuran mole fractions. However, with the exception of a few negative values seen at low 2-propanol mole fractions, the values of *n* for the mixture of 2-propanol and 2,2,4-trimethylpentane are positive. At T=298.15 K, n values range from -0.0034 to 0.0010. Tetrahydrofuran + 2-propanol + 2,2,4-trimethylpentane + 2-propanol = trimethylpentane. For each of these binary systems, the n values fall as the composition of mixture drops.The equation was used to connect the generated data, V^E,η, *n*, for ternary combinations of tetrahydrofuran (1) + 2-propanol (2) + 2, 2, 4-trimethylpentane(3) at 298.15 K;

$$\Delta Q_{123} = \Delta Q(x_1 x_2) + \Delta Q(x_1 x_3) + \Delta Q(x_2 x_3) + x_1 x_2 x_3 \sum_{i=0}^{2} \sum_{j=0}^{2-i} C_{ij} x_1^i x_2^j \tag{27}$$

where $x_3 = 1 - x_1 - x_2$ and Q_{123} refers to the physical characteristics of ternary mixes. According to the equation, *Q* represents the binary contribution functions for V^E,$\eta$and *n*. Using an optimization approach similar to the one used to obtain the binary parameters, the ternary parameters C_{ij} were calculated. Table 3 also includes the variables C_{ij} and related standard deviations.The experimental values of ternary V^E are positive at all compositions, as is expected from the behaviour of the binary mixtures (Figure 3). A composition at approximately *x*= 0.5 of 2-propanol results in the highest V^E value, which is found close to the 2-propanol + 2, 2, 4-trimethylpentane side. All ternary values are negative, with the lowest value occurring at a composition of roughly x= 0.6 of 2-propanol-propanol (2) + 2, 2, 4-trimethylpentane (3) at 298.15 K, close to the tetrahydrofuran + 2-propanol side.

5.Conclusion:

For the systems generated by tetrahydrofuran, 2-propanol, and 2, 2, 4-trimethylpentane at 298.15 K and atmospheric pressure over the whole composition range, this study presents experimental data on densities, viscosities, and refractive indices. All compositions have positive values for V^E, although most compositions have negative values for $\eta$and n. In terms of liquid mole fractions, the computed V^E, $\eta$and n, values were fitted to variable-degree polynomials. Except for Flory model, which was developed for non-electrolyte γ-meric spherical chain molecules and the systems under investigation have interacting and associating properties and Lorenz-Lorenz relation, as compared to others because of non-associated processes, theoretical dynamic viscosity, excess volume, and refractive index computed from various models agree well with the experimental value in all cases. However, the overall trend is essentially identical and favourable. The success of our experimental findings is supported by the very near values of the McAllister three- and four-body interaction models to the experimental data.

Acknowledgement:

Authorsare thankful to the staff of Department of Chemistry, BMM and V.S.S.D.College for support and cooperation

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