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Viscosity and Excess Viscosity for Associated Binary Mixtures at T= (298.15, 308.15 and 318.15)

Arun K.Singh, Brajesh Kumar and Rajeev K.Shukla*

Associate Professor*, Department of Chemistry, V.S.S.D.College, Kanpur-208002., India.*

email- rkshuklavssd@gmail.com

Vivek K.Pandey

Associate Professor, Department of Chemistry, D.B.S College, Kanpur, India

Abstract

Viscosities and excess viscosities for three binary systems (2-propanol + 2-phenylethanol) were computed at T= (298.15, 308.15, and 318.15) K over the concentration range 0.05-0.95 at atmospheric pressure and compared with the experimental work of Ching-Ta et al. Different theoretical models assuming association and non-association of the components of the mixtures, were used to predict the behavior of the studied liquids, which would typically show strong interactions. The properties were fitted to the Redlich-Kister polynomial equation to estimate the binary coefficients and standard errors. The excess viscosities were used to study the molecular interactions in the binary mixtures. Furthermore, the McAllister multi body interaction model was used to correlate the properties of the binary liquid mixtures. Testing of the models for the different systems showed that, compared with the non-association model theoretical results, the association model theoretical results were more consistent with the experimental results.

Keywords: Viscosity, Excess viscosity, Binary systems, Molecular interaction, Theoretical models

Introduction:

Viscosities are important basic data used in process simulation, equipment design, solution theory and molecular dynamics [1-2]. A better understanding of viscosity is of considerable physico-chemical interest and is essential in designing calculations involving heat transfer, mass transfer and fluid flow. Knowledge of viscosity is widely used in processing and product formulations [3] in many industrial applications. The paper is concerned with the mixing properties for two types of flavor alcohols, such as 2-phenylethanol mixed with 2-propanol. These alcohols are vitally related to our daily lives. 2-Phenylethanol is used in artificial essence and as a base solvent for some flavor compounds. 2-Propanol is a versatile solvent with protic and self-associated properties which can be used to study hydrophobic effects.

In this work, we present the theoretical results on viscosity and excess viscosity for binary system 2-propanol + 2-phenylethanol at T=(298.15,308.15,and 318.15) K over the concentration range 0.05-0.95 under atmospheric pressure. Several studies for binary mixtures involving 2-phenylethanol have been carried out in recent years [4-7] due to its nature of flavoring and forming association in the form of hydrogen bonds. To compare the merits of various models, the data were analyzed using the Ramaswamy and Anbananthan (RA) model [8], a model suggested by Glinski [9], McAllister multi body interactive model [10] and Flory model [11-12]. The first two of these models assume association of the components of the mixture, and include the association constant as an adjustable parameter. By contrast, the Flory model assumes the components do not associate (non-association), and that the behavior of each of the liquids in the mixture is simply additive when determining the overall properties. In the present study, we used liquids that usually show strong interactions. Changes in the viscosity, $\Delta\eta$ were evaluated and fitted to the Redlich-Kister polynomial [13] to derive the binary coefficients and standard errors. An attempt was made to correlate the experimental data with the McAllister multi body interaction model [10], based on Eyring's theory of absolute reaction rates [14]. The association behavior of the liquids was correlated with molecular interactions using the different liquid state models. Excess viscosities for all the three systems were calculated from the results of all the theoretical models used which is very much significant in understanding the nature and extent of molecular interactions involved in the liquid mixtures.

The main purpose of our work was to simulate various liquid state models which could describe the thermo-physical properties of all types of liquids well. For that purpose, we selected few binary liquids having strong association properties over the entire range of composition at various temperatures and applied associated and non-associated models simultaneously to study various thermo-physical properties. In the present work, the measured values of density and dynamic viscosity for these binary systems were taken from the work of Ching-Ta et al [15] and utilized for calculations.

Modeling:

RA Model:

Ramswamy and Anbananthan [8] proposed the model based on the assumption of linearity of acoustic impedance with the mole fraction of components. Assuming that when solute is added to solvent the molecules interact according to the equilibrium as:

$$A+B \leftrightarrow AB \qquad (1)$$

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

$$K_{as} = \frac{[AB]}{[A][B]} \qquad (2)$$

where [A] is amount of solvent and [B] is amount of solute in the liquid mixture.

By applying the condition of linearity in viscosity with composition

$$u_{obs} = x_A \eta_A + x_{AB} \eta_{AB} \qquad (3)$$

where x_A, x_{AB}, η_A and η_{AB} and η_{obs} are the mole fraction of A, mole fraction of associate AB, viscosity of A, viscosity of associate AB and observed viscosity respectively. The equilibrium reaction in the eq (3) is not complete by definition as there are molecules of non-associated component present in the liquid mixture prevailing in the high solute content. Considering the non-associated component present in the liquid mixture eq takes the fo

$$\eta_{RA} = [x_A \eta_A + x_B \eta_B + x_{AB} \eta_{AB}] \qquad (4)$$

where x_B and η_B are the mole fraction of B and viscosity of B (non-associated component).

The general idea of this model for predicting the values of pure associate AB can be, however, exploited as;

$$K_{as} = \frac{[AB]}{(C_A - [AB])(C_B - [AB])} \qquad (5)$$

where C_A and C_B are initial molar concentrations of the components. One can take any value of K_{as} and calculate the equilibrium value of [AB] for every composition of the mixture as well as [A] $=C_A$-[AB] and [B] $=C_B$-[AB]. Replacing molar concentration by activities for concentrated solution, eq (6) becomes,

$$K_{as} = \frac{a_{AB}}{(a_A - a_{AB})(a_B - a_{AB})} \quad (6)$$

where a_A, a_B and a_{AB} are the activity of component A, Component B and associate, AB respectively. Taking equimolar activities which are equal to; $a'_A = a_A - a_{AB}$ and $a'_B = a_B - a_A$

where a'_A and a'_B are the activities of [A] and [B] in equi molar quantities respectively.

From eq (6) one can obtain the value of K_{as} as; $K_{as} = \frac{a_{AB}}{a_A a_B - a_A a_{AB} - a_B a_{AB} + a_{AB}^2}$ (7)

Now, assuming any value of viscosity in the hypothetical pure component AB, η_{AB}, it is possible to compare the viscosity calculated using eq (4) with the experimental values. On changing both the adjustable parameters K_{as} and η_{AB} gradually, one can get different values of the sum of squares of deviations,

$$S = \Sigma\, (\eta_{obs} - \eta_{cal})^2 \quad (8)$$

where η_{obs} and η_{cal} are the observed and calculated viscosity respectively.

The minimum value of S can be obtained theoretically by a pair of the fitted parameters, but we found that for some K_{as} and η_{AB}, the value of S is high and changes rapidly while for others, it is low and changes slowly when the fitted parameters are being changed. In such cases, the value of η_{AB} should not be much lower than the lowest observed acoustic velocity of the system or much higher than the highest one. Quantitatively, it should be reasonable to accept the pair of adjustable parameters K_{as} and η_{AB} which has the physical sense and reproduces the experimental physical property satisfactorily.

Model Suggested by Glinski:

On inspecting the results obtained from RA model, Glisnki [9] suggested the equation assuming additivity with the volume fraction, ϕ of the components, the refined version of Natta and Baccaredda model [16] as,

$$\eta_{Glinski} = \frac{\eta_A \eta_B \eta_{AB}}{\phi_A \eta_B \eta_{AB} + \phi_B \eta_A \eta_{AB} + \phi_{AB} \eta_A \eta_B} \quad (9)$$

where η_{cal} is the theoretical acoustic velocity of binary liquid mixture, ϕ_A, ϕ_B are the volume fractions of component A and B and η_A, η_B and η_{AB} are the acoustic velocity of components A, B and AB. The numerical procedure and determination of association constant, K_{as}, was similar to that described before and the advantage of this method as compared with the earlier one was that the data on densities of liquid mixture are not necessary except those of pure components needed to calculate the volume fractions. In this context the importance of models assuming associated liquids already mentioned and was further developed and elaborated by Reis et al [17].

Flory model:

Theories relate the viscosities of liquids either to the activation energy required for the molecule to overcome the attraction forces of its neighbors and flow to a new position absolute rate theory) or the probability that an empty site exists near a molecule (free volume theory). Mecedo and Litovitz [18] made the hypothesis that the two effects are combined so that the probabilities for viscous flow is taken as the product of the probabilities for acquiring sufficient activation energy and of the occurrence of an empty site. Similar assumptions are made for solutions. A bridge can be formed to the thermodynamic functions of mixing by assuming a simple relationship between solution activation energy $\Delta G^{\neq}$, the pure liquid activation energy $\Delta G_1^{\neq}$, and the residual Gibbs free energy of mixing ΔG_M^R.

$$\Delta G^{\neq} = X_1 \Delta G_1^{\neq} + X_2 \Delta G_2^{\neq} - \Delta G_M^R \qquad (10)$$

For pure components and the solution the viscosities η_i are described as:

$$\eta_i = A \exp\left[\Delta G_1^{\#} / RT + (\tilde{V}_1 - 1)^{-1}\right] \qquad (11)$$

where $\tilde{V}_1$ is the reduced volume, Taking logarithms,

$$\ln \eta_i = \ln A + \frac{\Delta G_1{}^{\#}}{RT} + (\tilde{V}_1 - 1)^{-1} \qquad (12)$$

Applying eq. (12) to the solution and pure component, one obtains

$$\Delta \ln \eta = \ln \eta_{sol} - (X_1 \ln \eta_1 + X_2 \ln \eta_2) \qquad (13)$$

By utilizing eqs. (10) (11) and (13),the values of ΔG_M^R was evaluated from consideration of Flory theory and may be expressed as follows,

$$\Delta G_M^R = X_1 P_1^* V_1^* \left[\left(\frac{1}{\tilde{V}_1} - \frac{1}{\tilde{V}}\right) + 3\tilde{T}_1 \ln \frac{(\tilde{V}_1^{1/3} - 1)}{(\tilde{V}^{1/3} - 1)}\right]$$

$$+ X_2 P_2^* V_2^* \left[\left(\frac{1}{\tilde{V}_2} - \frac{1}{\tilde{V}}\right) + 3\tilde{T}_2 \ln \frac{(\tilde{V}_2^{1/3} - 1)}{(\tilde{V}^{1/3} - 1)}\right]^+$$

$$\frac{X_1 P_1^* V_1^* \theta_2 X_{12}}{\tilde{V}_1} \qquad (14)$$

By combining the Eyring [14] relation for the residual Gibbs free energy of mixing, ΔG^R_M and $\Delta G^{\#}$, we have obtained the following expression for the viscosity η of a binary liquid system:

$$RT \ln \eta = \sum_{i=}^{2} x_i \ln \eta_i - \left[\sum_{i=1}^{2} x_i P_i^* v_i^* \left\{(1/\tilde{v}_i - 1/\tilde{v}) + \right.\right.$$

$$3\tilde{T}_i \ln\left(\frac{(\tilde{v}^{1/3} - 1)}{(\tilde{v} - 1)}\right)$$

$$= \sum_{i=1}^{2} \sum_{j=1}^{2} (x_i v_i^* \theta_j x_{ij} / \tilde{v}_i) / RT \left(\frac{1}{\tilde{v} - 1}\right) - \left(\sum_{i=1}^{2} \frac{x_i}{\tilde{v} - 1}\right)$$

(15)

Here, P^*, v^*,$\tilde{v}$, $\tilde{T}$, θ and X_{ij} are the characteristic pressure, characteristic volume, reduced volume, reduced temperature, site fraction and interaction parameter respectively. All the notations in the above equation have their usual significance as detailed out by Flory [13-14] and others [19-20].

McAllister – three body model:

Eyring [14] gave the following equation relating kinematic viscosity of a liquid with to temperature

$$\partial = \frac{hN}{M} e^{\Delta G^{*}/RT^{\#}} \quad (16)$$

The movement of the molecule between two layers of liquid may be regarded as the passage of the system over a potential energy burrier, related to *ΔG** .McAllister considered a number of different three bodied planar encounters in the study of the viscosity of a mixture of molecules type (1) and (2). He proposed that the total free energy of activation will be dependent on thefree energy of activation (ΔG_i, ΔG_{ij} *or* Δs_{ijk}) of individual interactions and their fraction of total occurrences ($x_i^3, x_i^2 x_j, x_j^2, x_i x_j^2$ or $x_i x_j x_k$).Hence,

$$\Delta G^{*} = x_1^2 \Delta G_1^{*} + x_1^2 x_2 \Delta G_{121}^{*} + 2x_1^2 x_2 \Delta G_{112}^{*} + x_1 x_2^2 \Delta G_{212}^{*}$$

$$+ 2x_1 x_2^2 \Delta G_{123}^{*} + x_2^3 \Delta G_2^{*} \quad (17)$$

He made following additional assumptions as

$$\Delta G_{121}^{*} = \Delta G_{112}^{*} \equiv \Delta G_{12}^{*} \text{ and } \Delta G_{121}^{*} = \Delta G_{122}^{*} = \Delta G_{21}^{*}$$

Also, $\Delta G_{12}^{*} = \dfrac{\Delta G_{121}^{*} + 2\Delta G_{112}^{*}}{3}$ and $\Delta G_{21}^{*} = \dfrac{\Delta G_{212}^{*} + 2\Delta G_{122}^{*}}{3}$ (18)

Hence eq. (17) may written as

$$\Delta G^{*} = x_1^3 \Delta G_1^{*} + 3x_1^2 x_2 \Delta G_{12}^{*} + 3x_1 x_2^2 \Delta G_{21}^{*} + x_2^3 \Delta G_2^{*} \quad (19)$$

Now applying eq (17) for each set of interactions (i.e.*111,121,211, 112; 212, 122, 221; and 222*) and then taking logarithms of equations so obtained to eliminate free energy terms, following equation is obtained

$$\ln \eta = x_1^3 \ln \eta_1 + 3x_1^2 x_2 \ln \eta_{12} + 3x_1 x_2 \ln \eta_{21}$$
$$+ x_2^3 \ln \eta_2 - \ln[x_1 + x_2 M_2 / M_1] + 3x_1^2 x_2 \ln[(2 + M_2/M_1)/3]$$
$$+ 3x_1 x_2^2 \ln[(1 + 2M_2/M_1)/3] + x_2^3 \ln[M_2/M_1] \quad (20)$$

where $M_{12} = \dfrac{2M_1 + M_2}{3}$ and $M_{21} = \dfrac{M_1 + 2M_2}{3}$ (21)

McAllister –four body model:

If there is a much difference in size of two molecules, then a four body model approaches nearly a 3-dimensional treatment. Again considering different interactions and their fraction of total occurrences, energy of activation may be written as sum of energy of activations of various interaction $\Delta G^{*} = x_1^4 \Delta G_1^{*} + 4x_1^3 x_2 \Delta G_{1112}^{*} + 6x_1^2 x_2^2 \Delta G_{112}^{*} + 4x_1 x_2^3 \Delta G_{2221}^{*} + x_2^4 \Delta G_2^{*}$ (22)

by techniques entirely analogous to method given above, the following equation is derived;

$$\ln \eta_{mix} = x_1^4 \ln \eta_1 + 4x_1^3 x_2 \ln \eta_{1112} + 6x_1^2 x_2 \ln \eta_{1122}$$

$$+ 4x_1 x_2^2 \ln \eta_{222} + x_2^4 \ln \eta_2 - \ln(x_1 + x_2 M_2 / M_1)$$

$$+ 4x_1^3 x_2 \ln[(3 + M_2/M_1)/4] + 6x_1^2 x_2^2 \ln[(1 + M_2/M_1)/2]$$
$$+ 4x_1 x_2^3 \ln[(1 + 3M_2/M_1)/4] + x_2^4 \ln(M_2/M_1) \quad (23)$$

where η, x_1, η_1, M_1, x_2, η_2 and M_2 are the viscosity of mixture, mole fraction, viscosity and molecular weight of pure component 1 and 2 respectively. McAllister coefficients are adjustable parameters that are characteristic of the system.

Results and Discussion:

Association properties are usually evaluated using the deviation from the result that would be expected if the properties of the components were treated in an additive manner. The RA model, which assumes linearity of acoustic impedance with the amount-of-substance fraction of components, was used to derive a model that was corrected [9] and tested [21] to predict the behavior of each mixture with association between the components. The calculations were performed using a computer program, and the parameters were adjusted either automatically or manually. The association constant (*Kas*) and $\eta_{A,B}$ were used as the fitted parameters, where $\eta_{A,B}$ is the acoustic velocity in a hypothetical pure liquid with only the species AB formed by association of the components A and B. When the parameters are changed, the equilibrium concentrations of the species [A], [B], and [AB] will change and this could affect the viscosity. The differences between experimental and theoretical viscosity values were used to obtain sum of squares for the deviation. It was assumed that three species (A, B, and AB) were present in solution instead of only two (A and B) because of formation of the AB species by association after mixing. The acoustic velocity in the pure associate could be treated as a fitted one with a value of *Kas*.

Thermal expansion coefficient (α) and isothermal compressibility (β_T) values for the Flory model were obtained using an established equation, which has been tested on many mixtures [22]. The mixing function $(\Delta\sigma)$ can be represented mathematically by the Redlich-Kister polynomial [13] for correlating experimental data:

$$y = x_i(1-x_1)\sum_{i=0}^{p} A_i(2x_1-1)^i \tag{24}$$

where y is the change in viscosity $(\Delta\eta)$, x_i is the amount-of-substance fraction, and A_i is the coefficient. The values of the coefficients are summarized along with the standard deviations between the experimental and fitted values of the respective function (Table 1). For the dynamic viscosity, the range was 0.005-0.011.

Table 1 Coefficients of Redlich- Kister Polynomial and Standard Deviation (σ) for Viscosity of Binary Liquid Mixtures at Various Temperatures

2-Propenol+2-Phenylethnol

T/K	**A_0**	**A_1**	**A_2**	**A_3**	**Std dev. (σ)**
298.15	-5.35	0.81	-0.44	-0.81	0.008
308.15	-3.49	0.34	0.02	-0.19	0.009
318.15	-2.00	0.09	0.17	-0.19	0.011

McAllister coefficients a, b and c were calculated and standard deviations between the calculated and experimental values were determined (Table 2)

Table 2 Parameters of McAllister three body and four Body Interaction Models and Standard Deviation (δ) for Viscosity of Binary Liquid Mixtures at Various Temperatures

2-Propenol+2-Phenylethanol

Mc Allister Three Body				Mc Allister 4 body			
T/K	**a**	**b**	**Std dev**	**a**	**b**	**c**	**Std dev**
298.15	4.90	**7.84**	0.084	4.05	6.31	8.29	0.038
308.15	3.29	5.25	0.029	2.75	4.29	5.45	0.029
318.15	2.52	3.83	0.014	2.09	3.23	3.91	0.040

Excess viscosity was calculated by the following equation;

$$\eta E = \eta - \sum_{i=1}^{2} xi\,\eta i \qquad (25)$$

where η^E is excess viscosity is theoretical viscosity, η_i is viscosity for i th component and x_i amount-of-substance fraction for i th component.

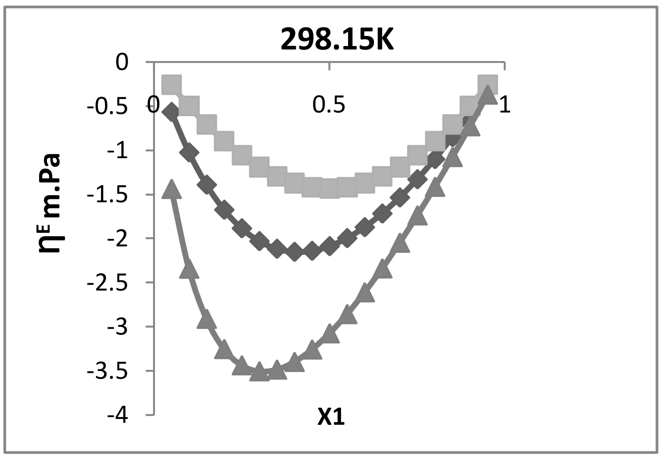
The data for the liquid mixtures (Tables 3-4) were evaluated.

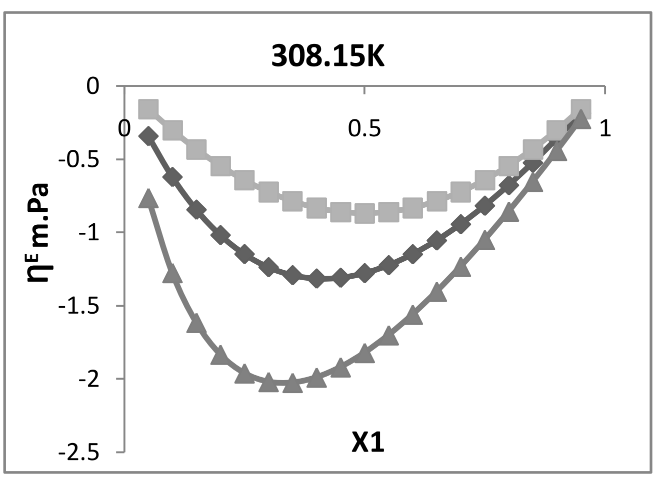
Table 3 Comparison of Absolute Average Percent Deviation of Viscosity obtained from Various Theoretical Models for Binary Liquid mixtures at (T=298.15, 308.15 and 318.15) K

2-Propenol+2-Phenyl ethanol

			Absolute Average % deviation				
T/K	**K_{as}**	**η_{ab}/mPa.s**	**η Flory/mPa.s**	**η RS/mPa.s**	**$\eta_{Glinski}$/mPa.s**	**η McA-3body /mPa.s**	**η McA-4body /mPa.s**
298.15	0.90	2.10	9.53	1.23	23.84	1.23	0.51
308.15	0.80	1.65	7.75	0.47	19.17	0.59	0.56
318.15	0.70	2.50	8.93	2.06	12.96	0.39	1.08

As the amount-of-substance fraction increased, the viscosity and excess viscosity decreased for all models at most temperatures, with a few exceptions. The absolute average percent deviations in the viscosity was calculated for the different models (Table 4). Models assuming association gave better results than those assuming non-association. Higher deviation for the values obtained by the Flory model could occur because this model was developed for non-electrolyte γ-meric spherical chain molecules, whereas the system under investigation in the present study will show interactions and association. Moreover, the expressions used for the computation of α and βT are empirical in nature. Negative deviations occur because of strong interactions and association. The actual sign and magnitude of the deviations depends upon the relative strengths of these two opposite effects. The lack of smoothness in the deviations arises from interaction between the component molecules. The viscosity values and excess viscosity values obtained from the different models (Table 4), and the percent deviations, indicate that our theoretical results are consistent with the experimental findings. Plots were constructed of changes in viscosity, η^E with the amount-of-substance fraction at various temperatures using different models (Figures 1).





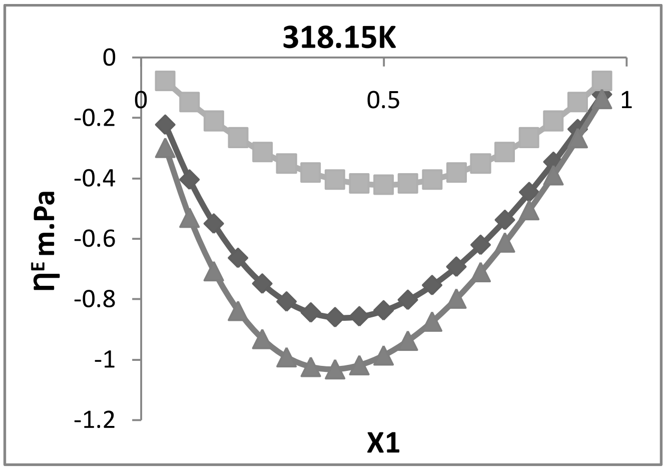


Figure 1 Changes in the excess viscosity *(η^E)* with the amount-of-substance fraction (x_1) for 2-propanol + (1–x) 2-phenylethanol at 298.15, 308.15 and 318.15 K. Results were obtained using the following models: black diamond, Flory model, black square, Ramaswamy and Anbananthan model, and black triangle, model suggested by Glinski

In all the cases, the association models showed lower changes in the excess viscosity than the non-association model (i.e. Flory model). The RA model gave better results than the model suggested by Glinski. The trends observed in all the figures were similar and showed negative changes with increasing temperature, which indicates stronger interactions between the liquid molecules at higher temperatures. Excess viscosity, η^E values are negative over the entire mole fraction range for all three binary mixtures. The results of excess viscosity at other temperatures follow the same trends. The values of η^E increases from T= 298.15K to T=318.15K for all these binary systems.

Conclusion:

Models assuming association give more reliable results than those assuming non-association. Association models can be helpful for determining how components in a mixture associate. This can be achieved using the viscosity in a hypothetical pure component and the observed dependence of concentration on the composition of a mixture.

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Table 4 Experimental Density, Experimental Viscosity, Theoretical Viscosity from Flory Model, Ramaswami and Anbananthan Model (RS),Model Devised by Glinski, McAllister 3 body (McA-3) and McAllister 4 body (McA-4) models and their Percent deviations for Binary Liquid Systems at various temperatures

2-Propenol+2-Phenyl ethanol

X1	ρ_{mix} g/cc	η_{exp} /mPa.s	ηFlory /mPa.s	η_{RS} / mPa.s	$\eta_{Glinski}$/ mPa.s	McA-3body/ mPa.s/	McA-4body/ mPa.s	%ΔFlory/ mPa.s	%Δ_{RS}/ mPa.s	%$\Delta_{Glinski}$/ mPa.s	%ΔMcA-3body/ mPa.s	%ΔMcA-4body/ mPa.s
T=298.15K												
0.05	1.0094	10.67	10.37	10.68	9.50	10.60	10.55	2.73	-0.14	10.90	0.60	1.08
0.10	1.0021	9.93	9.45	9.98	8.13	10.00	9.92	4.88	-0.44	18.13	-0.64	0.14
0.15	0.9944	9.26	8.61	9.30	7.10	9.41	9.33	6.93	-0.45	23.32	-1.67	-0.75
0.20	0.9864	8.62	7.86	8.64	6.29	8.84	8.76	8.74	-0.30	27.03	-2.63	-1.67
0.25	0.9780	8.00	7.19	8.02	5.64	8.30	8.22	10.16	-0.20	29.52	-3.73	-2.80
0.30	0.9691	7.41	6.58	7.42	5.10	7.77	7.71	11.22	-0.12	31.09	-4.94	-4.08
0.35	0.9599	6.86	6.02	6.84	4.66	7.27	7.22	12.18	0.19	32.08	-5.98	-5.21
0.40	0.9502	6.35	5.52	6.30	4.28	6.79	6.74	13.05	0.75	32.62	-6.86	-6.16
0.45	0.9400	5.86	5.07	5.79	3.95	6.32	6.29	13.56	1.22	32.57	-7.89	-7.25
0.50	0.9293	5.41	4.65	5.31	3.67	5.89	5.85	14.00	1.90	32.19	-8.75	-8.12
0.55	0.9180	4.98	4.28	4.86	3.42	5.47	5.44	14.05	2.40	31.26	-9.86	-9.20
0.60	0.9062	4.57	3.94	4.44	3.20	5.07	5.04	13.86	2.91	29.94	-11.00	-10.28

0.65	0.8936	4.17	3.63	4.05	3.01	4.70	4.67	13.11	3.00	27.93	-12.65	-11.83
0.70	0.8804	3.79	3.34	3.69	2.83	4.35	4.31	11.89	2.80	25.30	-14.66	-13.73
0.75	0.8663	3.44	3.08	3.35	2.68	4.02	3.98	10.33	2.42	22.16	-16.89	-15.84
0.80	0.8513	3.10	2.85	3.05	2.53	3.71	3.67	8.22	1.64	18.28	-19.60	-18.48
0.85	0.8355	2.81	2.63	2.77	2.41	3.42	3.39	6.36	1.29	14.34	-21.76	-20.66
0.90	0.8186	2.54	2.43	2.52	2.29	3.15	3.12	4.34	0.88	9.96	-23.93	-22.97
0.95	0.8005	2.28	2.25	2.29	2.18	2.90	2.88	1.41	-0.36	4.40	-27.05	-26.43
T=308.15K												
0.05	1.0023	7.05	6.88	7.06	6.47	7.05	7.00	2.45	-0.16	8.44	0.01	0.76
0.10	0.9949	6.59	6.30	6.62	5.66	6.66	6.58	4.46	-0.38	14.40	-0.93	0.26
0.15	0.9868	6.15	5.78	6.19	5.02	6.27	6.19	6.02	-0.71	18.57	-2.04	-0.62
0.20	0.9787	5.73	5.31	5.78	4.51	5.90	5.82	7.34	-0.93	21.57	-3.12	-1.65
0.25	0.9702	5.34	4.88	5.38	4.08	5.55	5.47	8.67	-0.79	23.89	-3.90	-2.49
0.30	0.9613	4.97	4.49	5.00	3.72	5.21	5.14	9.65	-0.71	25.39	-4.83	-3.53
0.35	0.9520	4.62	4.14	4.64	3.42	4.88	4.83	10.49	-0.46	26.35	-5.68	-4.51
0.40	0.9423	4.29	3.82	4.30	3.16	4.57	4.53	10.98	-0.29	26.72	-6.71	-5.65
0.45	0.9321	3.96	3.52	3.97	2.93	4.28	4.24	11.14	-0.22	26.53	-7.94	-6.95
0.50	0.9213	3.67	3.26	3.66	2.72	4.00	3.96	11.30	0.14	26.11	-8.98	-8.01
0.55	0.9100	3.39	3.01	3.38	2.54	3.74	3.70	11.15	0.39	25.22	-10.23	-9.23

0.60	0.8981	3.12	2.79	3.10	2.38	3.49	3.45	10.76	0.61	23.93	-11.63	-10.52
0.65	0.8855	2.88	2.58	2.85	2.24	3.25	3.22	10.17	0.83	22.30	-13.13	-11.88
0.70	0.8721	2.63	2.40	2.62	2.11	3.03	3.00	9.03	0.64	20.00	-15.22	-13.79
0.75	0.8580	2.41	2.22	2.40	2.00	2.83	2.79	7.60	0.32	17.25	-17.59	-15.99
0.80	0.8430	2.20	2.07	2.20	1.89	2.64	2.60	6.13	0.11	14.27	-19.93	-18.22
0.85	0.8270	2.01	1.92	2.01	1.79	2.46	2.43	4.39	-0.25	10.83	-22.57	-20.88
0.90	0.8101	1.86	1.79	1.84	1.71	2.30	2.27	3.87	0.77	8.34	-23.62	-22.16
0.95	0.7920	1.69	1.66	1.69	1.62	2.15	2.13	1.73	0.15	4.09	-26.78	-25.83
T=318.15K												
0.05	0.9942	4.95	4.81	4.95	6.45	4.97	4.93	2.94	0.01	4.46	-0.40	0.48
0.10	0.9868	4.65	4.42	4.68	5.64	4.72	4.66	4.78	-0.75	7.48	-1.69	-0.28
0.15	0.9790	4.37	4.07	4.41	5.01	4.48	4.41	6.68	-1.11	10.26	-2.61	-0.94
0.20	0.9708	4.10	3.76	4.16	4.49	4.24	4.17	8.41	-1.31	12.65	-3.40	-1.67
0.25	0.9623	3.85	3.47	3.91	4.06	4.01	3.95	9.86	-1.48	14.59	-4.21	-2.55
0.30	0.9534	3.60	3.21	3.67	3.71	3.79	3.73	10.88	-1.82	15.96	-5.25	-3.72
0.35	0.9440	3.36	2.97	3.43	3.40	3.57	3.53	11.68	-2.09	16.99	-6.30	-4.91
0.40	0.9342	3.13	2.75	3.21	3.14	3.37	3.33	12.16	-2.42	17.61	-7.49	-6.24
0.45	0.9239	2.91	2.55	2.99	2.91	3.17	3.13	12.37	-2.75	17.88	-8.78	-7.62
0.50	0.9131	2.71	2.37	2.78	2.71	2.98	2.95	12.68	-2.65	18.13	-9.74	-8.60

0.55	0.9017	2.52	2.20	2.59	2.53	2.80	2.77	12.79	-2.49	18.09	-10.76	-9.58
0.60	0.8897	2.34	2.05	2.40	2.38	2.62	2.59	12.58	-2.37	17.68	-11.98	-10.68
0.65	0.8770	2.16	1.91	2.22	2.23	2.46	2.43	11.84	-2.54	16.66	-13.71	-12.23
0.70	0.8636	1.99	1.78	2.04	2.11	2.30	2.27	10.72	-2.81	15.19	-15.78	-14.09
0.75	0.8494	1.82	1.66	1.88	1.99	2.16	2.12	9.16	-3.20	13.19	-18.27	-16.38
0.80	0.8343	1.67	1.55	1.73	1.89	2.02	1.98	7.18	-3.66	10.68	-21.19	-19.16
0.85	0.8183	1.53	1.44	1.58	1.79	1.89	1.86	5.42	-3.45	8.24	-23.71	-21.70
0.90	0.8013	1.42	1.35	1.44	1.70	1.77	1.74	4.66	-1.68	6.66	-24.82	-23.09
0.95	0.7831	1.30	1.26	1.31	1.62	1.65	1.64	2.79	-0.65	3.86	-27.31	-26.20