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Measurement and Calculation of Physico-Chemical Properties of Binary Mixtures Containing Xylene and 1-Alkanol

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ABSTRACT

Measured densities and viscosities of xylene, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol and 1-octanol and their binary mixtures with xylene in the liquid state were reported over the whole composition range at 298.15 K and atmospheric pressure. Regarding the experimental data, excess molar volumes and deviations in viscosity were calculated and interpreted in terms of intermolecular interactions and structural effects. Statistical association fluid theory (SAFT) and perturbed chain statistical association fluid theory (PC-SAFT) were applied to correlate the densities of binary mixtures. These models not only can accurately predict the density but also can obtain values by the PC-SAFT which are closely matched with the experimental data.

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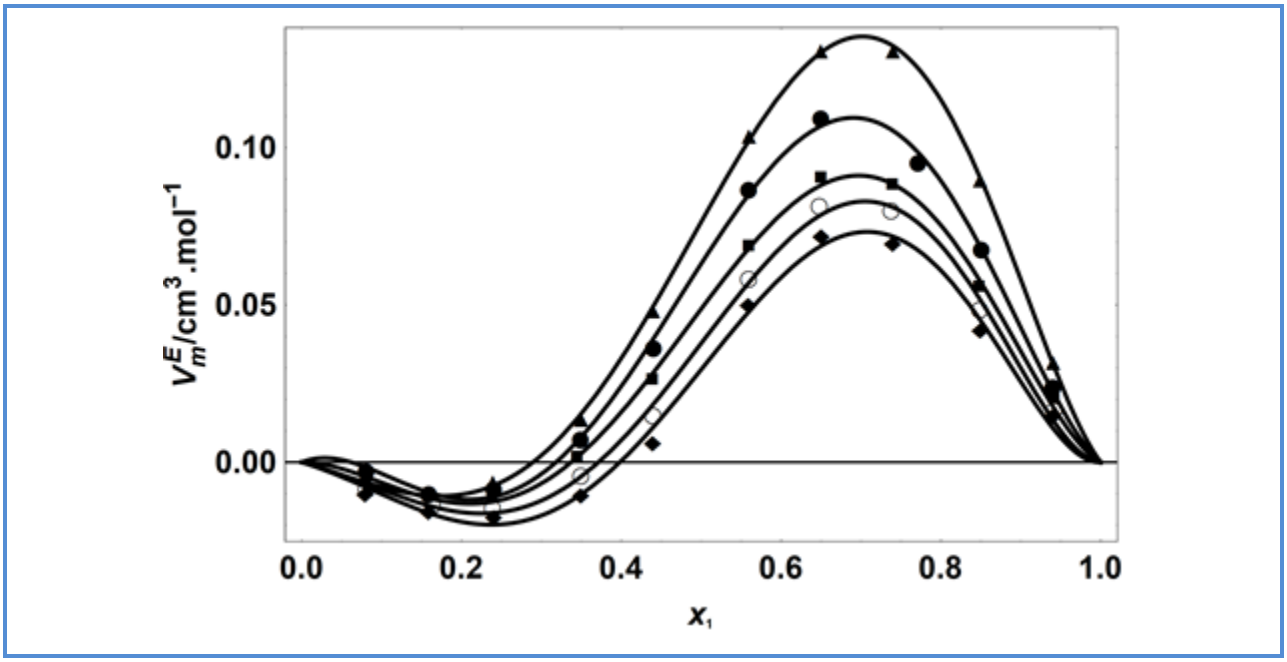
Graphical Abstract



Introduction

The densities and excess molar volumes of the investigated liquids and their mixtures are required, for instance, for relating excess enthalpy and excess Gibbs free energy values. From a practical point of view, the data are useful for the design of mixing, storage, and process equipment. Our studies are directed to investigate non-aqueous binary mixtures by physico-chemical properties [1-4] to provide useful informations about the molecular interactions. The density, viscosity and related properties of the xylene and 1-alkanol binary systems are reported here. Because of the presence of active sites for molecular interactions in both components, it is expected that the macroscopic behaviour of their binary mixtures may be related to these molecular features and interaction network. Therefore, this study aims to understand the intermolecular interactions between the xylene and 1-alkanol with differing hydrocarbon chain length. In recent years, the development and application of predictive models over a wide temperature range are extended. Recently, Gross and Sadowski have developed a new variation of the statistical association fluid (SAFT) theory called PC-SAFT. At present time, PC-SAFT is the most used version of the SAFT EOS. The correlative abilities of the SAFT and PC-SAFT models were tested in order to calculate the densities of binary mixtures.

Experimental

The used xylene, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol and 1-octanol were purchased from Merck and were used without further purifications. The mass fraction purities for all materials are greater than 99%. Density and viscosity were measured with a totally automated SVM 3000 Anton-Paar Stabinger viscometer that operates based on a modified Couette principle with a rapidly rotating outer tube and an inner measuring bob which rotates more slowly. A set of ten compositions was prepared for each mixture and their physical properties were measured at various compositions in the mole fraction range. The expanded uncertainty is 1×10^{-3} g·cm^{-3} for density measurements and the relative expanded uncertainty for viscosity measurements is 0.02. The estimated uncertainty in the mole fraction was $\pm1\times10^{-3}$.

Results and discussion

Densities and excess molar volumes

Densities and viscosities for pure compounds and their binary mixtures at various temperatures are reported in Table 2. The excess molar volumes, V_m^E were calculated using

$$V_m^E = \sum_{i=1}^{N} x_i M_i (\rho^{-1} - \rho_i^{-1}) \quad (1)$$

where x_i is the mole fraction, M_i is the molar mass of component i, ρ is the density of the mixture, ρ_i is the density of pure component i, and N stands for the number of components in the mixture. Figure 1 illustrates the graphs of excess molar volumes of xylene + 1-alkanol mixtures at T = 298.15 K. As this Figure shows, the excess molar volumes for all binary mixtures are positive in the whole composition range. Generally, V_m^E can be considered as arising from three types of interactions between component molecules. Physical interactions mainly consist of dispersion forces or weak dipole-dipole interactions and making a positive contribution. Chemical or specific interactions which include charge transfer, formation of hydrogen bonds and other complex forming interactions result in negative contribution. The positive deviation of V_m^E for xylene (1) + 1-alkanol (2) solvent system is governed by steric hindrances of molecules which overcome the other effect due to specific interactions between different species. In all the systems, the excess molar volume values are obviously increased with increasing the chain length of 2-alkanol. When the number of carbon atoms in the hydrocarbon part of 1-alkanol increases, the polar characteristics start

reducing which resist the formation of intermolecular interactions between xylene and 1-alkanol and hence the tendency to form associated complex decreases with the lengthening of carbon chain.

Dynamic Viscosities

The viscosity deviation can be calculated as

$$\Delta\eta = \eta - x_1\eta_1 - x_2\eta_2 \qquad (2)$$

where η is the mixture viscosity, η_1 and η_2 are the viscosities of pure components. Values of viscosity deviations were correlated by the Redlich– Kister equation. Figure 2 indicates the viscosity deviations for binary mixtures xylene + 1-alkanol at *T*=298.15 K. This figure shows that the viscosity deviations are negative for all binary mixtures over the entire mole fraction range and become more negative with increasing chain length of the alcohols.

SAFT Model

In this model, [5, 6] assumed that the liquid consists of equal-sized hard spheres, then, in order to account the attraction between the spheres, a dispersive potential is added. Next, to form the chains, two (or more) 'sticky' spots are given to the spheres. In the last step, at the certain position of chain, specific interaction sites are considered. Existence of these sites will enable the chains to associate through the attractive interaction like hydrogen bonding.

PC-SAFT Model

In the PC-SAFT model [7,8], a general expression for the residual Helmholtz energy is given by

$$a^{res} = a^{hc} + a^{dis} + a^{assoc} \qquad (3)$$

a^{hc} is the hard-sphere chain contribution, a^{dis} is dispersion interactions contribution and a^{assoc} is the association effects. Details of SAFT and PC-SAFT equations are mentioned elsewhere and are not provided here.

SAFT and PC-SAFT models were used to correlate the density values. Table 2 lists the correlation parameters for binary mixtures evaluated by application of mentioned models. Two models yielded small AAD and provided good correlations. By contrast, the PC-SAFT model provides more accurate values for densities and more agreement with experimental data.

Table 1. Densities *ñ* and viscosities η for the binary mixtures at 298.15 and pressure *P*=0.1 MPa.

T/K = 298.15					
Densities(ρ /g·cm^{-3}) for Xylene +					
x_1	1-Butanol	1-Pentanol	1-Hexanol	1-Heptanol	1-Octanol
0	0.8055	0.8108	0.8151	0.8187	0.8214
0.081	0.811	0.815	0.8184	0.8213	0.8236
0.1595	0.8159	0.8189	0.8217	0.8242	0.8262
0.2395	0.8207	0.8229	0.825	0.827	0.829
0.3501	0.8268	0.8279	0.8295	0.8311	0.8328
0.4397	0.8313	0.8317	0.833	0.8344	0.8361
0.5601	0.8369	0.8364	0.8379	0.839	0.8406
0.6497	0.8409	0.84	0.8417	0.8423	0.8436
0.7404	0.8449	0.8453	0.845	0.8458	0.8465
0.8492	0.8498	0.8492	0.8497	0.8498	0.8501
0.9407	0.8539	0.8536	0.8538	0.853	0.8534
1	0.8564	0.8564	0.8564	0.8564	0.8564
Viscosities (η /mPa.s)					
0	2.5807	3.4925	4.5845	5.9242	7.6182
0.081	2.1504	2.8535	3.6899	4.61	6.0051
0.1595	1.7822	2.3272	2.9719	3.63	4.8687
0.2395	1.5025	1.9078	2.42051	2.9469	3.7803
0.3501	1.17	1.4733	1.85	2.2148	2.7297
0.4397	1.027	1.2382	1.4754	1.783	2.1538
0.5601	0.8681	0.9789	1.12	1.2874	1.5804
0.6497	0.772	0.8448	0.9558	1.0925	1.263
0.7404	0.7188	0.7324	0.853	0.9397	1.0213
0.8492	0.6702	0.6956	0.7211	0.7673	0.7785
0.9407	0.6481	0.6688	0.6465	0.6588	0.6791
1	0.624	0.624	0.624	0.624	0.624

Table 2. Binary Interaction Parameter k_{ij} and standard deviation σ for SAFT and PC-SAFT Equations

			k_{ij}	%σ
Binary Systems	**SAFT**	**PC-SAFT**	**SAFT**	**PC-SAFT**
Xylene + 1-Butanol	0.025	0.012	1.32	1.08
Xylene + 1-Pentanol	0.054	0.018	1.23	1.06
Xylene + 1-Hexanol	0.066	0.023	1.43	1.14
Xylene + 1-Heptanol	0.068	0.028	1.56	1.18
Xylene + 1-Octanol	0.084	0.032	1.73	1.15

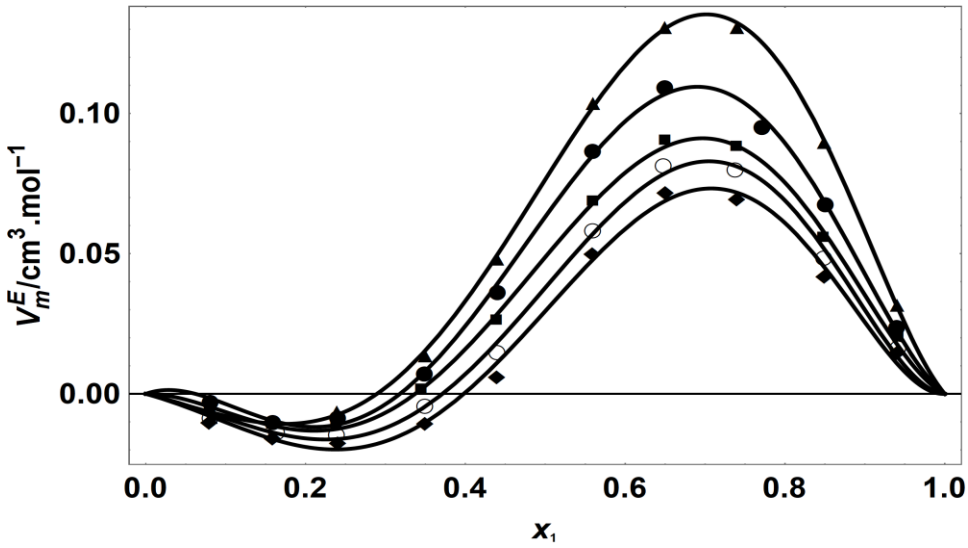


Figure 1. Excess molar volumes V_m^E vs. mole fraction of xylene for binary mixtures of xylene with (♦) 1-butanol, (○)1-pentanol, (■)1-hexanol, (●)1-heptanol, (▲) 1-octanol, 2-pentanol at T = 298.15 K.

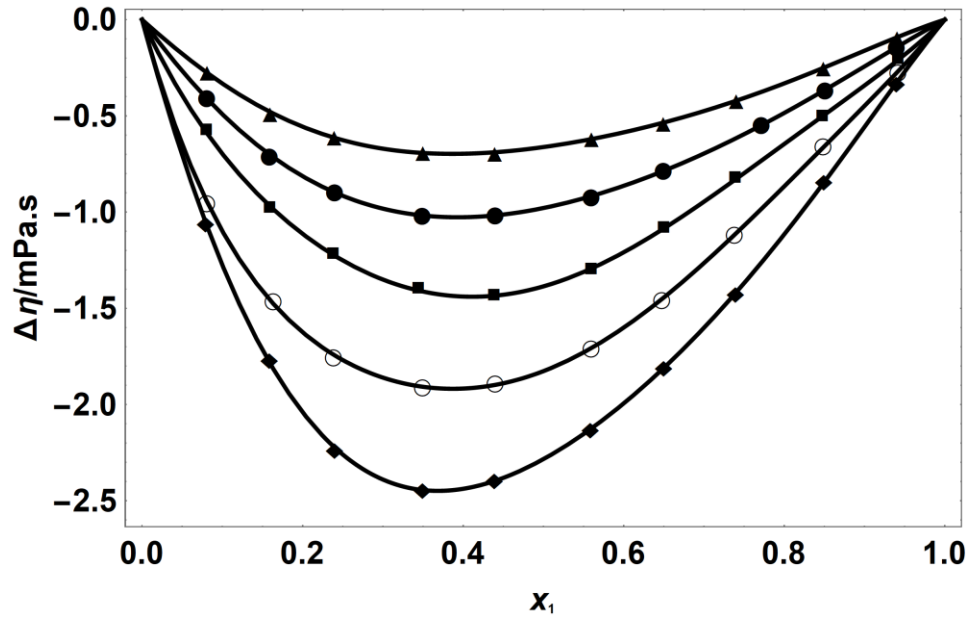


Figure 2. Viscosity deviations Δη vs. mole fraction of xylene for binary mixtures of xylene with (▲) 1-butanol , (●)1-pentanol, (■)1-hexanol, (○)1-heptanol, (♦) 1-octanol, 2-pentanol at T = 298.15 K.

Conclusion

Densities and viscosities for binary mixtures consisting xylene + 2-alkanol were measured and the corresponding excess molar volumes and viscosity deviations have been calculated. Excess molar volumes are positive and viscosity deviations are negative for all the studied mixtures. The structure of xylene /alcohol mixtures is governed by hindrances effects in the carbon chain of

alcohols. Two models namely SAFT and PC-SAFT were applied to correlate the densities of binary liquid mixtures and, as a result, they yielded low AAD for correlation of density. However, the predicted values by PC-SAFT are more accurate.

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