Using Properties of Binary Liquid Mixtures on Statistical Mechanical Theories

Dr. K. G. Neerajakshi

Department of Chemistry, The Adoni Arts & Science College, Adoni, Kurnool, India.

Abstract

Thermodynamic properties of liquids and liquid mixtures play very important role in understanding the nature of molecular interactions occurring in the system. In the present work different thermodynamic properties of 15 pure liquids and 34 equimolar binary liquid mixtures of benzene, toluene, p-xylene, chlorobenzene and 1-chloronaphthalene with linear and branched alkanes have been computed with the help of Flory's statistical theory (FST), Hard sphere equation of state (HSE) and Hole theory (HT) simultaneously. The calculated values are compared with the experimental findings collected from literature and quite satisfactory results are obtained.

Keywords: *Flory statistical theory; hard sphere equation of state; hole theory; binary liquid mixtures.*

1. Introduction

During the recent past it has been customary to utilize ultrasonic velocity data for the computation of a number of interesting and useful equilibrium and transport properties of liquids and liquid mixtures (Acosta et al., 2001; Dhasi et al., 1998; Ali & Tiwari et al., 2000; Mosteriro et al., 2001; Ali & Nain, 2002; Baluja, 2002; Ali & Ahmad et al., 2000; Arce et al., 2000; Canosa et al., 2001). Since velocity and density measurements are quite simple and economical, such studies are useful in estimating these properties. Also, some of the properties which cannot be determined directly from the experimental method, they can be obtained from velocity and density data. On the other hand, several empirical and semi-empirical procedures (Nomoto, 1958; Van Dael, 1975; Jakobson, 1951; Schaffs, 1939; Jain et al., 1974; Kaulgud & Patil, 1972; Acree (Jr), 1984; Reid et al., 1987; Rowlinson & Swinton, 1982; Murrell & Jenkins, 1982; Prausnitz et al., 1986; Eyring & John, 1969; Pandeyet al., 1997; Pandey et al., 1999; Pandey & Vyas et al., 1999; Ali & Nain, 2000; Ali & Nain, 2002) have also been used to estimate theoretically the sound velocity. Due to the importance of ultrasonic velocity, various liquid state models have been employed successfully to correlate this property with other, and also a theoretical evaluation has been carried out. It would be interesting to mention some liquid state models e.g. Flory's statistical theory (FST) (Flory et al., 1964; Flory, 1965; Abe & Flory, 1965; Bloomfeld & Dewan, 1971; Dewan et al., 1971; Pandey & Alec David, 1981; Pandey & Sanguri, 2008; Pandey & Sanguri, 2001; Pandey & Sanguri et al., 2002; Pandey & Sanguri et al., 2003; Dey & Pandey et al., 2006), Hard sphere equation of state (HSE) (Percus & Yevick, 1958; Lebowitz et al., 1965; Thiele, 1963; Lebowitz & Frisch et al., 1961; Carnahan & Starling, 1969; Frisch, 1964; Hoover & Ree, 1964) and Hole theory (HT) (Pandey & Sanguri et al., 2010; Pandey & Sanguri et al., 2007; Pandey, Dwivedi & Sanguri, 2008; Sanguri et al., 2008), that were utilized to deduce ultrasonic velocity and other thermodynamic properties of liquids and liquid mixtures (binary and higher orders). A comparative study of the applicability of various liquid state theories employed for the estimation of thermodynamic and other related properties has, so far, not been done. An entirely different procedure has been adopted in the present work. The present work has the following merits:

(i) To make a comparative study of Flory's statistical theory (FST), Hard sphere equation of state (HSE) andHole theory (HT) on the basis of theoretically computed values of various thermodynamic properties of 15 pure liquids and 34 equimolar binary liquid mixtures.

(ii) An attempt has been made to evaluate ultrasonic velocities in the above mentioned systems from the experimental values of thermal expansivity (α), heatcapacity at constant pressure (C_P) and isothermal compressibility (β_T). These values of sonic velocities are treated as experimental values.

(iii) These experimentally deduced values of velocity are compared with the theoretical ones obtained from FST and HT.

(iv) Nine different physical properties (viz. β_T, β_S, α, C_P, C_V, P_i, γ, Γ and u) are theoretically calculated by FST and HT and compared with the experimental findings.

(v) α and β_T are also calculated with the help of seven different HSE and compared with the experimental values.

(vi) Theoretical estimation of the density of equimolar binary mixtures has been done with the help of FST.

These studies are made by using the typical experimental data of Tardajos & Patterson et al., 1986;

Costas & Patterson et al., 1988; Dominguez & Patterson et al., 1993. Such types of data are very rare in the literature. They measured quite accurately and precisely molarvolume (V), thermal pressure coefficient (γ_P), thermal expansivity, isothermal compressibility and heat capacity at constant pressure of 15 pure liquids and their binary mixtures. In the present work, we are applying FST, HSE and HT for estimating the values of various thermodynamic properties of 15 pure liquids and 34 equimolar binary liquid mixtures of benzene, toluene, p-xylene, chlorobenzene, and 1-chloronaphthalene with linear (n-C_6, n-C_8, n-C_{10}, n-C_{12}, , n-C_{14} & n-C_{16}) and branched alkanes (br- C_6, br-C_8, br-C_{12} and br-C_{16}). As far as our knowledge is concerned, this is for the first time, when three very important liquid state theories (viz. FST, HSE and HT) are simultaneously employed for the estimation of physical properties of liquids and liquid mixtures.

2. Theoretical

Flory theory, HSE and HT have been recently (Flory et al., 1964; Flory, 1965; Abe & Flory, 1965; Bloomfeld & Dewan, 1971; Dewan et al., 1971; Pandey & Alec David, 1981; Pandey & Sanguri, 2008; Pandey & Sanguri, 2001; Pandey & Sanguri, 2002; Pandey & Sanguri, 2003; Dey & Pandey, 2006; Percus & Yevick, 1958; Lebowitz et al., 1965; Thiele, 1963; Lebowitz & Frisch et al., 1961; Carnahan & Starling, 1969; Frisch, 1964; Hoover & Ree, 1964; Pandey & Sanguri et al., 2010; Pandey & Sanguri et al., 2007; Pandey, Dwivedi & Sanguri, 2008; Sanguri et al., 2008) utilized for computing various thermodynamic and transport properties of liquid mixtures. Variousmodifications of FST have been made and utilized successfully. The relevant equations are summarized here. The details of these equations are given in earlier papers (Pandey & Sanguri, 2008; Pandey & Sanguri, 2001; Pandey& Sanguri et al., 2002; Pandey & Sanguri et al., 2003; Dey & Pandey, 2006 et al., 2006).

The equilibrium properties of a liquid are strongly

Thermal expansivity, density (ρ), isothermal compressibility, internal pressure (P_i), heat capacity at constant pressure, adiabatic compressibility (β_s), ultrasonic velocity (u), heat capacity ratio (γ), heat capacity at constant volume (C_V) and Gruneisen parameter (Γ) by Flory theory are calculated with the help of following equations:

$$\alpha = \frac{\left(\tilde{V}^{1/3} - 1\right)}{T\left(1 - 3\left(\tilde{V}^{1/3} - 1\right)\right)} \quad (1)$$

$$\rho = \frac{x_1 M_1 + x_2 M_2}{\left(x_1 V_1^* + x_2 V_2^*\right)\tilde{V}} \quad (2)$$

$$\beta_T = \frac{\alpha^2 \tilde{V} T}{P^*} \quad (3)$$

$$P_i = \frac{\alpha T}{\beta_T} \quad (4)$$

$$C_P = \left(x_1 C_{P,1} + x_2 C_{P,2}\right) + C^E_P \quad (5)$$

$$\beta_S = \beta_T - \frac{\alpha^2 T V}{C_P} \quad (6)$$

$$u = \left(\frac{1}{\beta_S \rho}\right)^{1/2} \quad (7)$$

$$\gamma = \left.\frac{\beta_T}{\beta_S}\right| \quad (8)$$

$$C_V = \left.\frac{C_P}{\gamma}\right| \quad (9)$$

$$\Gamma = \frac{\gamma - 1}{\alpha T} \quad (10)$$

dependent on what may be loosely called its local structure, often expressed in terms such as packing density, free volume or, more exactly, in terms of the radial distribution function. Flory et al used a simple partition function proposed by Eyring & Hirschfelder to get the reduced equation of state, which is based on vander Waals potential energy model. They assume the intermolecular energy to depend only on the volume, and a hard sphere repulsive potential is adopted for segments of the chain. The number of external degree of freedom is introduced as a parameter on the premise that the corresponding modes can be separated unambiguously from the internal degrees of freedom of molecules. From the knowledge of α, β and V.

The basic idea of the hole theory is to assume the existence of holes in liquid. A liquid can be treated as a solution of molecules and holes. The appearance of holes can be regarded as a particular case of hetrophase fluctuations. The holes can be treated as gas bubbles when these are large enough to accommodate a sufficient amount of vapours. Surface tension and internal pressure of pure liquid components are the only input data for estimating thehole radius, hole volume and hole creation energy in the present hole theory. From these three properties, it is possible to calculate various thermodynamic properties of liquids and liquid mixtures.

Isothermal compressibility, thermal expansivity and ultrasonic velocity of pure liquids by hole theory are calculated using the following equations:

The details of these equations and symbols are given in our earlier papers (Pandey & Sanguri et al., 2010; Pandey & Sanguri et al., 2007; Pandey, Dwivedi & Sanguri, 2008; Sanguri et al., 2008).

The equations used to calculate isothermal compressibility, thermal expansivity and ultrasonic velocity of binary mixtures by hole theory are analogous to theabove Eqs. (11), (12) and (13). Here we use molar volume of the mixture (V_{mix}), volume of a hole in the mixture ($V_{h\,(mix)}$) and energy of creation of a hole in the mixture ($E_{h\,(mix)}$) in place of V, V_h & E_h. The method of calculation of $V_{h\,(mix)}$ and $E_{h\,(mix)}$ is given in the literature (Pandey & Sanguri et al., 2007). With the help of calculated values of β_T, α and u by hole theory, we have also calculate β_S, C_P, γ, C_V using Eqs. (6), (7), (8), (9) and (10) respectively.

The equation of state proposed by vander Waals accounts in a remarkable manner for most essential featuresof fluid behaviour, it fails to give the accurate representation of experimental thermodynamic data required in practice. Therefore, many modifications of the equation have been proposed, which generally involve the introduction of a dependence of the parameter '**a**' and '**b**'

on temperature and or density. With the help of virial equation of state and hard sphere potential, hard sphere equation of state is obtained. Various theoretical

approaches have been suggested by different workers for

Table 1. The necessary data needed, for the calculation, have been taken from different sources (Tardajos & Patterson et al., 1986; Costas & Patterson et al., 1988; Dominguez & Patterson et al., 1993; CRC, 1997). Table 2 enlists the percentage deviations of different properties of pure components using hole theory and Flory theory. In Table 3, percentage deviations of different properties of binary mixtures calculated through Flory theory, have been presented. In the present work only percentage deviations of different properties have been reported. The computed values of the desired thermodynamic properties of pure components and binary liquid mixtures can be obtainedfrom the authors on request.

For the comparison of theoretically computed valueswith the observed values under consideration, the experimental values of liquid mixtures were taken fromdifferent sources (Tardajos & Patterson et al., 1986; Costas & Patterson et al., 1988; Dominguez & Patterson et al., 1993). The experimental values of ρ, β_S, γ, C_V, P_i and u of binary liquid mixtures were obtained by the following equations:

The basic idea of the hole theory is to assume the existence of holes in liquid. A liquid can be treated as a solution of molecules and holes. The appearance of holes can be regarded as a particular case of hetrophase fluctuations. The holes can be treated as gas bubbles when these are large enough to accommodate a sufficient amount of vapours. Surface tension and internal pressure of pure liquid components are the only input data for estimating thehole radius, hole volume and hole creation energy in the present hole theory. From these three properties, it is possible to calculate various thermodynamic properties of liquids and liquid mixtures.

Isothermal compressibility, thermal expansivity and ultrasonic velocity of pure liquids by hole theory are calculated using the following equations:

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The equations used to calculate isothermal compressibility, thermal expansivity and ultrasonic velocityof binary mixtures by hole theory are analogous to theabove Eqs. (11), (12) and (13). Here we use molar volume of the mixture (V_{mix}), volume of a hole in the mixture ($V_{h\,(mix)}$) and energy of creation of a hole in the mixture ($E_{h\,(mix)}$) in place of V, V_h & E_h. The method of calculation of $V_{h\,(mix)}$ and $E_{h\,(mix)}$ is given in the literature (Pandey & Sanguri et al., 2007). With the help of calculated values of

β_T, α and u by hole theory

$$\beta_{S_{exp}} = \frac{1}{u^2_{exp}\rho^{exp}}$$

Table 1. Different properties of pure components at 298.15 K

Component	V	$\alpha \times 10^3$ K^{-1}	$\tilde{V}$	V^*	$\tilde{T}$	T^*	$\beta_T \times 10^{12}$ $cm^2\ dyne^{-1}$	P^* $J\ cm^{-3}$	M	ρ	C_P $JK^{-1}mol^{-1}$
chlorobenzene	102.24	0.982	1.2440	82.1863	0.0564	5284.012	75.50	600.13	112.56	1.1009	153.78
1-chloronaphthalene	136.77	0.702	1.1833	115.5881	0.0461	6467.786	48.80	600.49	162.62	1.1890	212.60
n-C_6	131.563	1.381	1.3209	99.5987	0.0671	4444.85	166.90	430.46	86.18	0.6550	197.67
n-C_8	163.526	1.160	1.2796	127.7928	0.0617	4835.431	128.20	441.74	114.23	0.6985	254.07
n-C_{10}	195.92	1.041	1.2561	155.9808	0.0583	5117.714	109.40	447.59	142.28	0.7262	315.32
n-C_{12}	228.578	0.978	1.2432	183.8661	0.0563	5296.037	98.80	456.12	170.34	0.7452	376.09
n-C_{14}	261.339	0.931	1.2334	211.8878	0.0548	5445.317	91.00	464.02	198.39	0.7591	438.01
n-C_{16}	294.052	0.902	1.2273	239.6004	0.0538	5545.426	85.70	472.64	226.25	0.7694	500.21
br-C_6	133.697	1.460	1.3350	100.1495	0.0688	4335.187	198.20	391.41	86.18	0.6446	191.88
br-C_8	166.056	1.192	1.2858	129.1468	0.0625	4769.492	151.20	388.60	114.23	0.6879	242.49
br-C_{12}	229.621	0.977	1.2430	184.7358	0.0563	5299.059	113.80	395.47	170.34	0.7418	350.98
br-C_{16}	289.84	0.854	1.2170	238.1624	0.0521	5726.497	92.90	405.93	226.25	0.7806	458.80
benzene	89.408	1.218	1.2908	69.2677	0.0632	4718.574	96.60	626.32	78.12	0.8737	136.67
toluene	106.875	1.086	1.2651	84.4810	0.0596	5003.421	91.40	566.96	92.15	0.8622	158.67
p-xylene	123.923	1.019	1.2516	99.0126	0.0576	5177.397	84.40	563.88	106.17	0.8567	183.65

Table 2. Percentage deviation of different properties of pure components using Hole theory and Flory theory.

Component	%u (Flory theory)	%β_T	%β_S	%α	%C_P	%u
		(Hole theory)				
chlorobenzene	8.69	-11.81	-8.51	-11.87	47.63	15.96
1-chloronaphthalene	9.01	---	---	---	---	---
n-C_6	-5.93	7.19	9.03	7.11	49.88	6.74
n-C_8	-4.94	-5.66	-4.31	-5.74	34.86	11.54
n-C_{10}	-4.47	-5.59	-4.73	-5.67	26.41	10.88
n-C_{12}	-3.91	-2.04	-1.56	-2.11	18.92	9.09
n-C_{14}	-3.45	-17.11	-16.86	-17.18	-4.67	14.97
n-C_{16}	-2.98	-10.21	-10.21	-10.28	-10.47	12.30
br-C_6	-16.63	13.39	15.24	13.31	55.26	3.19
br-C_8	-6.81	-5.64	-4.01	-5.73	40.78	11.00
br-C_{12}	-5.56	---	---	---	---	---
br-C_{16}	-4.28	---	---	---	---	---
benzene	6.78	-4.63	-1.30	-4.69	48.42	15.76
toluene	4.24	-11.36	-8.34	-11.43	44.86	16.30
p-xylene	3.84	-16.25	-13.80	-16.31	36.37	17.66

Table 3. Percentage deviation of different properties of binary mixtures calculated through Flory theory

Components	x_1	$\%\beta_T$	$\%\beta_S$	$\%\alpha$	$\%C_P$	$\%P_i$	$\%\gamma$	$\%\rho$	%u	$\%\Gamma$	$\%C_V$
benzene(x_1) + n-C_6(x_2)	0.5000	3.26	3.72	-0.16	-1.79	-3.53	-0.48	-0.44	-1.69	-1.75	-1.30
benzene(x_1) + n-C_8(x_2)	0.5000	2.64	3.57	-0.83	-0.70	-3.57	-0.97	-0.46	-1.60	-3.37	0.27
benzene(x_1) + n-C_{10}(x_2)	0.5000	2.61	3.09	-0.63	-1.72	-3.32	-0.49	-0.42	-1.37	-1.66	-1.22
benzene(x_1) + n-C_{12}(x_2)	0.5000	2.05	2.84	-1.24	-0.97	-3.35	-0.82	-0.40	-1.25	-2.80	-0.15
benzene(x_1) + n-C_{14}(x_2)	0.5000	2.01		-2.05		-4.15		-0.38			
benzene(x_1) + n-C_{16}(x_2)	0.5000	2.03	3.12	-2.29	-1.44	-4.41	-1.13	-0.38	-1.41	-3.69	-0.31
toluene(x_1) + n-C_6(x_2)	0.5000	2.40	2.49	0.65	-0.60	-1.80	-0.09	-0.25	-1.14	-1.03	-0.51
toluene(x_1) + n-C_8(x_2)	0.5000	2.59	3.23	0.08	0.13	-2.57	-0.67	-0.23	-1.54	-3.16	0.80
toluene(x_1) + n-C_{10}(x_2)	0.5000	1.74	2.11	-0.21	-0.51	-1.98	-0.38	-0.21	-0.97	-1.64	-0.12
toluene(x_1) + n-C_{12}(x_2)	0.5000	1.77	2.21	-0.51	-0.84	-2.33	-0.44	-0.20	-1.02	-1.73	-0.39
toluene(x_1) + n-C_{14}(x_2)	0.5000	1.43		-0.86		-2.32		-0.13			
toluene(x_1) + n-C_{16}(x_2)	0.5000	1.24	1.85	-1.36	-1.13	-2.63	-0.62	-0.14	-0.86	-1.97	-0.51
p-xylene(x_1) + n-C_6(x_2)	0.5000	4.91	5.84	0.76	-0.11	-4.36	-0.98	-0.16	-2.97	-5.11	0.87
p-xylene(x_1) + n-C_{16}(x_2)	0.5000	2.60	3.42	-0.58	-0.04	-3.27	-0.85	-0.04	-1.74	-4.07	0.81
chlorobenzene(x_1) + n-C_6(x_2)	0.5000	2.10	2.02	0.98	-0.32	-1.14	0.08	-0.09	-0.98	-0.64	-0.40
chlorobenzene(x_1) + n-C_8(x_2)	0.5000	2.29	2.34	0.70	-0.62	-1.63	-0.05	-0.11	-1.13	-0.94	-0.57
chlorobenzene(x_1) + n-C_{10}(x_2)	0.5000	2.25	2.31	0.60	-0.70	-1.69	-0.06	-0.17	-1.09	-0.87	-0.64
chlorobenzene(x_1) + n-C_{12}(x_2)	0.5000	1.63	1.87	-0.15	-0.86	-1.81	-0.24	-0.12	-0.88	-1.06	-0.62
chlorobenzene(x_1) + n-C_{14}(x_2)	0.5000	1.87	2.15	-0.22	-0.95	-2.12	-0.29	-0.12	-1.03	-1.33	-0.66
chlorobenzene(x_1) + n-C_{16}(x_2)	0.5000	1.48	1.85	-0.63	-1.00	-2.14	-0.38	-0.08	-0.90	-1.44	-0.62
chlorobenzene(x_1) +br-C_6(x_2)	0.5000	1.43	1.61	0.24	-0.24	-1.21	-0.18	-0.13	-0.75	-1.01	-0.06
chlorobenzene(x_1) +br-C_8(x_2)	0.5000	1.45	1.62	0.27	-0.27	-1.19	-0.18	0.02	-0.83	-1.12	-0.09
chlorobenzene(x_1) + br-C_{12}(x_2)	0.5000	0.75	0.74	0.38	-0.05	-0.37	0.01	0.03	-0.39	-0.34	-0.06
chlorobenzene(x_1) +br-C_{16}(x_2)	0.5000	0.51	0.43	0.50	0.05	-0.01	0.08	0.06	-0.25	-0.05	-0.02
1-chloronaphthalene(x_1) + n-C_6(x_2)	0.5000	3.33	3.12	2.04	-0.08	-1.34	0.22	-0.04	-1.58	-0.99	-0.30
1-chloronaphthalene(x_1) + n-C_8(x_2)	0.5000	3.00	2.82	2.12	0.56	-0.91	0.18	-0.06	-1.41	-1.23	0.38
1-chloronaphthalene(x_1) + n-C_{10}(x_2)	0.5000	2.90	2.59	2.42	0.63	-0.50	0.32	-0.08	-1.28	-0.74	0.31
1-chloronaphthalene(x_1) + n-C_{12}(x_2)	0.5000	2.74	2.44	2.26	0.51	-0.49	0.30	-0.09	-1.20	-0.61	0.21
1-chloronaphthalene(x_1) + n-C_{14}(x_2)	0.5000	2.42	2.18	1.91	0.35	-0.52	0.25	-0.08	-1.07	-0.55	0.11
1-chloronaphthalene(x_1) + n-C_{16}(x_2)	0.5000	1.99	1.72	1.67	0.15	-0.33	0.27	-0.07	-0.84	-0.13	-0.13
1-chloronaphthalene(x_1) +br-C_6(x_2)	0.5000	3.95	4.52	0.86	0.28	-3.22	-0.59	-0.25	-2.21	-3.86	0.87
1-chloronaphthalene(x_1) + br-C_8(x_2)	0.5000	2.90	3.07	1.14	0.19	-1.81	-0.18	-0.08	-1.53	-2.10	0.36
1-chloronaphthalene(x_1) +br-C_{12}(x_2)	0.5000	2.35	2.48	0.82	0.02	-1.57	-0.13	-0.13	-1.20	-1.59	0.15
1-chloronaphthalene(x_1) +br-C_{16}(x_2)	0.5000	2.38	2.52	0.73	-0.07	-1.69	-0.15	-0.12	-1.22	-1.64	0.07

In the present work a number of useful and important properties of binary liquid mixtures have been theoretically estimated on the basis of Flory's statistical theory. The estimated properties are the thermal expansion coefficient, isothermal compressibility, adiabatic compressibility, heat capacity at constant pressure, internal pressure, density, heat capacity ratio, ultrasonic velocity, Gruneisen parameter and heat capacity at constant volume. Ultrasonic velocity is also calculated for pure components using Flory theory. Theoretically obtained values on the basis of a refined version of Flory theory developed by Pandey et al. (Pandey & Sanguri, 2008; Pandey & Sanguri, 2001; Pandey & Sanguri, 2002; Pandey & Sanguri, 2003; Dey & Pandey et al, 2006), are compared with the experimental findings. Itis clear from Table 2, that in general there is a good agreement between theoretical and experimental values of ultrasonic velocity of pure components. The maximum percentage deviation is -16.63% for br- C_6. In general the order of percentage deviation is about 3 to 5 percent. One of the reasons for slightly higher percentage deviation in 'u' is that we are using Auerbach empirical equation for the calculation of ultrasonic velocity for pure components. A close observation of Table 3 shows that the agreement between the experimental and theoretical values of all the estimated properties for all the systems is excellent. The maximum percentage deviation of each property is summarized below:

β_T	β_S	α	C_P	P_i	γ	ρ	u	Γ	C_V
4.91	5.84	2.42	1.79	4.41	0.98	0.46	2.97	5.11	1.30

Table 4 enlists the percentage deviations of different properties (viz. β_s, C_p, P_i, γ, Γ & C_v) of binary mixtures calculated with the help of hole theory. The percentage deviation in the values of β_T, α and u for the above

Table 4. Percentage deviation of different properties of binary mixtures calculated through Hole theory

Table 4. Percentage deviation of different properties of binary mixtures calculated through Hole theory

Components	% Deviation						
	x_1	$\%\beta_S$	$\%C_P$	$\%P_i$	$\%\gamma$	$\%\Gamma$	$\%C_V$
1-chloronaphthalene(x_1) + n-C_6(x_2)	0.5000	-2.57	43.75	16.32	-13.06	-68.13	50.25
1-chloronaphthalene(x_1) + n-C_8(x_2)	0.5000	0.05	-12.88	-2.28	2.28	11.52	-15.52
1-chloronaphthalene(x_1) + n-C_{10}(x_2)	0.5000	1.08	5.01	-0.91	-1.88	-8.15	6.77
1-chloronaphthalene(x_1) + n-C_{12}(x_2)	0.5000	1.53	16.36	2.01	-4.11	-21.86	19.66
1-chloronaphthalene(x_1) + n-C_{14}(x_2)	0.5000	1.50	20.00	0.58	-6.59	-32.35	24.95
1-chloronaphthalene(x_1) + n-C_{16}(x_2)	0.5000	1.13	18.45	-0.05	-6.67	-30.77	23.54
1-chloronaphthalene(x_1) +br-C_6(x_2)	0.5000	-2.49	37.67	13.26	-9.50	-52.01	43.08
1-chloronaphthalene(x_1) + br-C_8(x_2)	0.5000	-0.01	-35.35	-5.77	4.73	25.61	-42.06
1-chloronaphthalene(x_1) +br-C_{12}(x_2)	0.5000	2.19	8.58	3.14	-0.06	-5.87	8.63
1-chloronaphthalene(x_1) +br-C_{16}(x_2)	0.5000	2.76	-5.73	-1.04	1.42	5.91	-7.25
chlorobenzene(x_1) + n-C_6(x_2)	0.5000	3.30	-12.48	-9.59	-1.53	1.07	-10.78
chlorobenzene(x_1) + n-C_8(x_2)	0.5000	4.06	16.79	-1.80	-9.57	-34.05	24.06
chlorobenzene(x_1) + n-C_{10}(x_2)	0.5000	3.57	35.75	6.60	-15.15	-67.41	44.21
chlorobenzene(x_1) + n-C_{12}(x_2)	0.5000	2.44	56.40	21.12	-19.17	-115.63	63.42
chlorobenzene(x_1) + n-C_{14}(x_2)	0.5000	13.91	58.33	12.24	-25.64	-164.63	66.83
chlorobenzene(x_1) + n-C_{16}(x_2)	0.5000	0.71	58.99	21.08	-24.56	-139.71	67.08
chlorobenzene(x_1) +br-C_6(x_2)	0.5000	3.06	1.92	7.84	6.04	11.71	-4.38
chlorobenzene(x_1) +br-C_8(x_2)	0.5000	4.68	42.01	18.47	-3.79	-45.90	44.12
chlorobenzene(x_1) + br-C_{12}(x_2)	0.5000	1.24	49.92	18.54	-12.57	-83.11	55.51
chlorobenzene(x_1) +br-C_{16}(x_2)	0.5000	1.70	-4.20	-2.08	0.45	2.47	-4.67
benzene(x_1) + n-C_6(x_2)	0.5000	4.69	-49.97	-1.34	12.73	41.03	-71.85
benzene(x_1) + n-C_8(x_2)	0.5000	4.72	-34.78	-9.54	5.57	23.25	-42.73
benzene(x_1) + n-C_{10}(x_2)	0.5000	3.85	-13.03	-10.29	-1.34	1.12	-11.53
benzene(x_1) + n-C_{12}(x_2)	0.5000	2.86	30.82	5.07	-11.67	-53.24	38.05
benzene(x_1) + n-C_{14}(x_2)	0.5000	-1.87	22.26	3.31	-11.98	-39.26	30.57
benzene(x_1) + n-C_{16}(x_2)	0.5000	1.32	35.76	3.63	-18.74	-78.12	45.90
toluene(x_1) + n-C_6(x_2)	0.5000	3.38	-47.36	-10.18	7.74	31.02	-59.72
toluene(x_1) + n-C_8(x_2)	0.5000	4.93	9.64	-1.90	-3.93	-17.20	13.06
toluene(x_1) + n-C_{10}(x_2)	0.5000	3.77	25.33	1.88	-10.72	-45.49	32.56
toluene(x_1) + n-C_{12}(x_2)	0.5000	3.41	12.41	-3.73	-7.11	-26.84	18.22
toluene(x_1) + n-C_{14}(x_2)	0.5000	-0.15	29.88	8.87	-8.21	-40.64	35.20
toluene(x_1) + n-C_{16}(x_2)	0.5000	1.76	41.03	10.26	-13.18	-72.26	47.90
p-xylene(x_1) + n-C_6(x_2)	0.5000	-0.49	-38.56	-5.77	6.72	28.79	-48.53
p-xylene(x_1) + n-C_{16}(x_2)	0.5000	-1.08	48.03	14.49	-17.31	-93.01	55.70

3. Conclusion

The results obtained by applying FST, HSE and HT to the pure liquids and 34 equimolar binary mixtures at 298.15K are remarkable. Out of the ten properties of binary mixtures calculated by FST, the two most important properties viz. density and ultrasonic velocity give excellentagreement with the experimental findings collected from literature as the APD values are found to be in the order of 1% (in case of density) and below 2% (in case of ultrasonic velocity). In case of density, the maximum APD is found to be 0.46%. The APD values for the rest of the eightproperties are below 6% which is excellent.

In general, the percentage deviation is below 7% for β_s,P_i, and γ in case of Hole theory, whereas for C_P, C_V & Γ the percentage deviation is little higher. For β out of the seven Rest models give percentage deviations between HSE, only Guggenheim model gives some satisfactory results, other models are not found to be suitable for the calculation of β_T. In a few cases, Thiele-Lebowitz and Carnahan-Starling model gives satisfactory results. For thermal expansivity different types of trends are observed but in most of the cases Henderson model and Scaled-particle theory give satisfactory results. The above results have led to the conclusion that FST is superior in all respects to HSE and HT.

Since theoretically obtained values of density and ultrasonic velocity by FST have APD values below 1% and 2% respectively in the present work.

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