Experimental and Modeling Density and Surface Tension of 1, 2-Dimethylbenzene with Alkanes at 298.15K

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***Abstract*— *Experimental density and surface tension of 1,2-dimethylbenzene with octane, nonane and decane have been obtained at 298.15K and atmospheric pressure. This work increases the available experimental information regarding this kind of mixtures useful in the fuel field. The excess molar volume and the surface tension deviation have been correlated by Redlich-Kister polynomial equation. Besides, density of binary systems has been predicted and correlated with Nitta-Chao group contribution and ERAS models respectively while the surface tension deviation have been predicted with HSIS and HSEG and SE models. Finally, a comparison about the behavior of excess volume molar and deviation surface tension between dimethylbenzene isomers and alkanes is presented.*

***Keywords*— density, surface tension, 1,2-dimethylbenzene, alkane.**

I. INTRODUCTION

Methylbenzenes occur in small quantities in naphtha and higher boiling fractions of petroleum. Those presently of commercial importance are toluene, 1,2-dimethylbenzene (o-xylene), 1,4-dimethylbenzene (p-xylene), and to a much lesser extent 1,3-dimethylbenzene (m-xylene). Particularly, 1,2-dimethylbenzene is mainly used to produce phthalic anhydride for plasticizers. The primary sources of xylenes are reformates from catalytic reforming units, gasoline from catcraking, and pyrolysis gasoline from steam reforming of naphtha and gas oils. Solvent extraction is used to separate these aromatics from the reformate mixtures [1]. For this reason, physical properties of pure and mixtures liquids containing aromatic and aliphatic compounds and their dependence with composition are very important basic data for petrochemical industry.

Some experimental data of density and surface tension are available in literature for 1,4-dimethylbenzene and alkanes [2-4]. In this sense, in previous works we have also studied high pressure density for 1,4-dimethylbenzene pure component and its binary mixtures with dimethyl carbonate, diethyl carbonate, n-octane and n-decane at (288.15, 298.15 and 308.15) K and (0.1, 5, 10, 20, 30 and 40) MPa [5]. However, from our knowledge only a few experimental data about excess molar volume have been reported by Cáceres Alonso and Delgado[6] for 1,2-dimethylbenzene – octane binary mixtures, while excess molar volume and density have been reported by Cáceres Alonso and Delgado [6] and Chevalier et al.[7] respectively for 1,2-dimethylbenzene – decane binary mixtures. For this reason, in this work, experimental data of density and surface tension of 1,2-dimethylbenzene with octane, nonane and decane at 298.15K and atmospheric pressure are presented. These behaviors are compared with those showed by 1,4-dimethylbenzene and 1,3-dimethylbenzene with alkanes.

Redlich-Kister polynomial equation has been used to correlate the excess molar volume and the surface tension deviation. Moreover, Nitta-Chao group contribution and ERAS models have been used to predict and correlate the density data of dimethylbenzene – alkanes systems respectively, while, HSIS, HSEG and SE models have been used in the predictions of the surface tension deviation.

II. EXPERIMENTAL SECTION

Purity, supplier, CAS-number and physical properties such as density and surface tension at 298.15K of the compounds used in this work are presented in Table 1. These products have not had further purification. For comparison, experimental information available in the literature [8-26] is also presented in this table.

Pure components of binary mixtures were weighted in an AND HM 202 balance with an uncertainty of ±10^{-4} g. In this way, the uncertainty in the mole fractions of the prepared mixtures was estimated to be ± 0.0001.

TABLE 1
CAS-NUMBER, SUPPLIER, PURITY AND PHYSICAL PROPERTIES AT 298.15K OF STUDIED COMPOUNDS

				ρ / g.cm^{-3}		σ /mN.m^{-1}	
Chemical name	**CAS-number**	**Supplier**	*** Mole Fraction Purity**	**This work**	**Literature**	**This work**	**Literature**
octane	111-65-9	Fluka	≥ 0.995	0.69874	0.69855 [8] 0.6987 [9] 0.69845 [10]	21.01	20.99 [8] 21.14 [11] 21.19 [12]
nonane	111-84-2	Fluka	≥ 0.99	0.71394	0.71385 [13] 0.7139 [14] 0.713834 [15]	22.12	22.30[12] 22.49 [16] 22.37 [17]
decane	124-18-5	Fluka	≥ 0.98	0.72614	0.72609 [18] 0.7262 [9] 0.7260 [19]	23.10	23.39 [20] 23.26 [12] 23.10 [18]
1,2-Dimethylbenzene	95-47-6	Fluka	≥ 0.99	0.87551	0.87528 [21] 0.87550 [22] 0.8750 [23]	28.99	29.27 [24] 29.35 [25] 29.60 [26]

***Without further purification.**

Density measurements of binary mixtures and their respective pure compounds were carried out in a vibrating-tube Anton Paar DMA 4500 densimeter, with a density repeatability of 10^{-5} g.cm^{-3}. The densimeter temperature was reached and maintained through a PolyScience 9510 circulating fluid thermostatic bath and it was tested by a CKT-100 platinum probe with an uncertainty lower that 5.10^{-2} K. More details about the experimental technique can be found in earlier publications [27].

On the other hand, surface tension was determined using an automatic tensiometer Lauda TVT2 with a total accuracy of the surface tension determination better than 0.1 mN.m^{-1}. This property was assessed for both pure components and binary mixtures based on the principle of the pending drop volume. In this method, the volume of a drop falling from a capillary with a radius *r* is measured. The drop continuously grows by means of an accurate dosing system and it eventually detaches and a new drop starts to grow. The drop volume is measured during the time interval of droplet formation which is determined by a light barrier. The interfacial tension is calculated from the averaged volume measured for several subsequent drops formed at the same dosing rate. Thus, the surface tension is determined by the following equation:

$$\sigma = \frac{\Delta\rho g V}{2\pi \, \mathrm{r}_{cap} f} \tag{1}$$

where $\Delta\rho$ is the density difference between the liquid and vapor phase, g is the gravitational acceleration, V is the drop volume, $2r_{cap}$ is the outer diameter of the capillary, and f is a shape correction factor. The TVT2 software determines the correction factor f using a polynomial function proposed by Wilkinson [28].

Before each series of measurements the instrument was calibrated at atmospheric pressure with water Milli-Q and air.

Thus, density and surface tension were measured at 298.15 K and atmospheric pressure by duplicate and triplicate respectively for binary mixtures containing 1,2-dimethylbenzene with octane, nonane and decane. The average deviation and the maximum deviation for these three binary systems in density were 9.6x10^{-6} and 2.83 x10^{-5} and surface tension were 0.034 and 0.070 respectively.

Excess molar volumes V^E and surface tension deviations $\Delta\sigma$ were calculated from experimental values using the following expressions:

$$V^E = V_M - \sum_i x_i V_i \tag{2}$$

$$\Delta\sigma = \sigma_M - \sum_i x_i \sigma_i \tag{3}$$

where V_M and σ_M are molar volume of the mixture and surface tension and V_i and σ_i are the corresponding values for the pure component *i*.

Table 2 shows experimental density (ρ) and excess molar volume (V^E) and Table 3 shows surface tension (σ) and surface tension deviation ($\Delta\sigma$) of 1,2-dimethylbenzene with octane, nonane and decane at 298.15 K and atmospheric pressure.

TABLE 2
EXPERIMENTAL DENSITY (ρ) AND EXCESS MOLAR VOLUME (V^E) OF 1, 2-DIMETHYLBENZENE WITH OCTANE, NONANE AND DECANE AT 298.15 K AND ATMOSPHERIC PRESSURE.

x_1	ρ/g.cm^{-3}	V^E/ cm^3.mol^{-1}	x_1	ρ/g.cm^{-3}	V^E/ cm^3.mol^{-1}	x_1	ρ/g.cm^{-3}	V^E/cm^3.mol^{-1}
octane (x_1) + 1,2-dimethylbenzene (x_2)			**nonane (x_1) + 1,2-dimethylbenzene (x_2)**			**decane (x_1) + 1,2-dimethylbenzene (x_2)**		
0.0516	0.8635	-0.0033	0.0499	0.8637	0.0172	0.0585	0.8616	0.0382
0.1041	0.8516	-0.0116	0.1006	0.8523	0.0301	0.1023	0.8519	0.0601
0.1993	0.8312	-0.0209	0.1984	0.8319	0.0481	0.2058	0.8308	0.1015
0.3004	0.8108	-0.0238	0.2996	0.8125	0.0604	0.3049	0.8128	0.1267
0.4016	0.7917	-0.0259	0.4007	0.7947	0.0752	0.4022	0.7970	0.1429
0.5992	0.7574	-0.0107	0.4960	0.7792	0.0881	0.5012	0.7823	0.1503
0.7991	0.7265	0.0009	0.6015	0.7634	0.0857	0.6010	0.7689	0.1484
0.8995	0.7123	0.0021	0.6986	0.7500	0.0742	0.6944	0.7575	0.1323
0.9475	0.7057	0.0011	0.7952	0.7376	0.0610	0.8007	0.7457	0.1034
			0.8974	0.7254	0.0373	0.8982	0.7357	0.0599
			0.9489	0.7195	0.0187	0.9497	0.7308	0.0324

The average and the maximum standard deviation in density for all measurements are 9.6x10^{-6} and 2.83 x10^{-5} respectively. The uncertainty of the variables are: u(T)= 5.10^{-2} K; u(x_1)= ± 10^{-4}; u(ρ) =10^{-4} g.cm^{-3}; and the combined expanded uncertainty with level of confidence 0.95 (k = 2) for the density is: $U_c(\rho)$= 2. 10^{-4} g.cm^{-3}.

TABLE 3
EXPERIMENTAL SURFACE TENSION (σ) AND SURFACE TENSION DEVIATION ($\Delta\sigma$) OF 1,2-DIMETHYLBENZENE WITH OCTANE, NONANE AND DECANE AT 298.15 K AND ATMOSPHERIC PRESSURE.

x_1	σ /mN.m^{-1}	$\Delta\sigma$/mN.m^{-1}	x_1	σ /mN.m^{-1}	$\Delta\sigma$/mN.m^{-1}	x_1	σ /mN.m^{-1}	$\Delta\sigma$/mN.m^{-1}
octane (x_1) + 1,2-dimethylbenzene (x_2)			**nonane (x_1) + 1,2-dimethylbenzene (x_2)**			**decane (x_1) + 1,2-dimethylbenzene (x_2)**		
0.0503	28.05	-0.545	0.0501	28.13	-0.522	0.0500	28.13	-0.569
0.0996	26.89	-1.311	0.0979	27.43	-0.893	0.0993	27.49	-0.921
0.2002	25.85	-1.542	0.1994	26.28	-1.346	0.1990	26.52	-1.301
0.3016	24.89	-1.695	0.2990	25.36	-1.582	0.2977	25.84	-1.402
0.4021	24.07	-1.711	0.4005	24.73	-1.514	0.3995	25.23	-1.409
0.5054	23.35	-1.605	0.5040	24.10	-1.427	0.4995	24.69	-1.356
0.6032	22.80	-1.378	0.6021	23.64	-1.220	0.5995	24.32	-1.137
0.7036	22.26	-1.117	0.7017	23.13	-1.038	0.7012	23.91	-0.948
0.8016	21.86	-0.731	0.7986	22.77	-0.731	0.8008	23.56	-0.718
0.9062	21.33	-0.426	0.9003	22.42	-0.382	0.9022	23.31	-0.367
0.9501	21.23	-0.175	0.9499	22.19	-0.278	0.9492	23.30	-0.104

The average and the maximum standard deviation in surface tension for all measurements are 0.034 and 0.070 respectively. The uncertainty of the variables are: u(T)= 5.10^{-2} K; u(x_1)= ± 10^{-4}; u(σ)= 0.1 mN.m^{-1}; and the combined expanded uncertainty with level of confidence 0.95 (k = 2) for the superficial tension is: $U_c(\sigma)$= 0.2 mN.m^{-1}.

III. DENSITY AND SURFACE TENSION MODELING

Calculated data of excess molar volume V^E and surface tension deviation $\Delta\sigma$ were correlated with composition data by Redlich-Kister polynomial [29], which for binary mixtures is

$$Q_{ij} = x_i x_j \sum_k A_k \left(x_i - x_j\right)^k \tag{4}$$

where Q_{ij} is V^E or $\Delta\sigma$, x_i is the mole fraction of component i, A_k is the polynomial coefficient obtained by least-squares regression, and k is the number of the polynomial coefficient defined by Fisher's F-test. These results can be seen in Table 4.

TABLE 4
REDLICH-KISTER COEFFICIENTS AND STANDARD DEVIATIONS S FOR EXCESS MOLAR VOLUME V^E OBTAINED FOR FITS OF EQ. 4 IN THE INVESTIGATED SYSTEMS AT 298.15 K.

A_0/ cm^3.mol^{-1}	A_1/ cm^3.mol^{-1}	A_2/ cm^3.mol^{-1}	A_3/ cm^3.mol^{-1}	SD/cm^3.mol^{-1}
octane (x_1) + 1,2-Dimethylbenzene (x_2)				
-0.0765	0.1480	0.0482	-0.1012	0.0009
nonane (x_1) + 1,2-Dimethylbenzene (x_2)				
0.3373	0.0641	-	-	0.0027
decane (x_1) + 1,2-Dimethylbenzene (x_2)				
0.6145	0.0206	-	-	0.0030

Nitta-Chao group contribution model [30] based on the cell theory with the repulsive forces between molecules has been applied to the density and the excess volume for the family of dimethylbenzene with alkane binary mixtures. More details about this model and the group definition of the molecules studied in this work can be found in Gayol et al. [5] Table 5 presents the parameters involved in this kind of mixture.

TABLE 5
NITTA-CHAO PARAMETERS INVOLVED IN THE DENSITY OF 1,2 DIMETHYLBENZENE WITH ALKANES BINARY MIXTURES[5]

Pure group								
Group	$V_{i,0}^{*}/\left(cm^3.mol^{-1}\right)$			a_i / **K**		c_i		Q_i
$-CH_3$	13.46			23.7		0.338		6.71
$-CH_2$	10.25			23.7		0.093		4.27
$-CH_{ar}$	7.98			33.28		0.174		3.13
$-C_{ar\text{-}al}$	4.70			33.28		-0.127		0.95

Binary parameters				
i	***j***	$\varepsilon_{ij} = \varepsilon_{ji}$ / **(J.mol^{-1})**	$\sigma_{ij}^{0} = \sigma_{ji}^{0}$ / **(J.mol^{-1})**	$\sigma_{ij}^{'} = \sigma_{ji}^{'}$ / **(J.mol^{-1})**
$-CH_3$	$-CH_3$	2515	0	0
	$-CH_2$	2515	0	0
	$-CH_{ar}$	3276	0	0
	$-C_{ar\text{-}al}$	3276	0	0
$-CH_2$	$-CH_2$	2515	0	0
	$-CH_{ar}$	3276	0	0
	$-C_{ar\text{-}al}$	3276	0	0
$-CH_{ar}$	$-CH_{ar}$	4284	0	0
	$-C_{ar\text{-}al}$	4284	0	0
$-C_{ar\text{-}al}$	$-C_{ar\text{-}al}$	4284	0	0

Furthermore, VE has been correlated using a simplified Extended Real Associated Solution model (ERAS) [31]. According to Bender and Heintz[32], the excess molar volume can be thought to be composed of two additive components: a physical and a chemical contribution. Some authors [33-34], found that only physical contribution represents very well the V^E behaviour. This is especially true for non-polar mixtures taking into account that physical contribution terms is based on Flory's equation of state [35] which consider the free volume effects of liquids and liquid mixtures of nonpolar molecules of different size and shape. For this reason, in this work a simplified ERAS model taking into account only physical terms is applied to correlate the V^E of 1,2 dimethylbenzene –alkanes mixtures. Details about this model and the equations used can be found in Tôrres et al. [33] Table 6 resume the ERAS parameters involved in the pure compounds and binary mixtures studied in this work [18, 31, 36-39].

TABLE 6
ERAS PARAMETERS FOR DENSITY OF DIMETHYLBENZENE ISOMERS WITH ALKANES BINARY MIXTURES

Pure component	**ρ g.cm^{-3}**	**σ mN.m^{-1}**	***10^4x α (1/K)***	***10^4 x κ_T (1/MPa)***	***Δv_i^* (cm^3/mol)***	***Δh_i^* (kJ/mol)***	***K_i***	***S_i (1/nm)***
1,2 dimethylbenzene	0.87551[a]	28.99[a]	9.52[b]	8.10 [b]	-3.00 [b]	-15.0 [b]	0.13 [b]	12.51*
1,3 dimethylbenzene	0.85978[c]	28.03 [c]	9.81[b]	8.62 [b]	- 8.00 [b]	-15.0 [b]	0.14 [b]	12.51*
1,4 dimethylbenzene	0.8566 [d]	27.43[d]	9.56 [b]	8.59 [b]	- 8.00 [b]	-15.0 [b]	0.12 [b]	12.51 [e]
n-octane	0.69874[a]	21.01[a]	11.64 [f]	12.82 [f]	-	-	-	13.91 [f]
n-nonane	0.71394[a]	22.12 [a]	10.83 [g]	11.71 [g]	-	-	-	13.82 [g]
n-decane	0.72614[a]	23.10 [a]	10.44 [f]	11.42[f]	-	-	-	13.78 [f]
Binary System			***χ_{AB} (J/cm^3)***	***SD***				
1,2 dimethylbenzene/n-octane			11.68	0.0038				
1,2 dimethylbenzene/n-nonane			12.65	0.0045				
1,2 dimethylbenzene/n-decane			13.24	0.0063				
1,3 dimethylbenzene/n-octane			10.02	0.0045				
1,4 dimethylbenzene/n-octane			7.34	0.0021				

[a] This work; [b] Ref. [36]; [c] Ref. [37]; [d] Ref. [18]; [e]. Ref. [38]; [f] Ref. [39]; [g] Ref. [31]; * No literature data was found and the S value was supposed equal to the 1,4 dimethylbenzene.

On the other hand, surface tension and surface tension deviation were predicted using different theoretical models. Specifically, we apply the theories of Hildebrand and Scott [40] for ideal solutions (HSIS) and their extension of Guggenheim's ideal solution equation (HSEG) [40], useful for systems containing molecules of significantly different size and the Sudgen's equation based on the parachor (SE) [41]. A summary of the three models and their equations is exposed in Domínguez-Pérez et al. [24].

Standard deviation SD has been included in Tables 4, 6-8 in order to evaluate the efficiency of the modeling in excess molar volume and surface tension deviation by the following equation:

$$SD = \sqrt{\sum_{i}^{N}\left(Q_{ij}^{\exp} - Q_{ij}^{cal}\right)^2 / N} \tag{5}$$

where *Qij* is *V*E or Δσ, where N is the number of experimental data, *exp*: experimental data and *cal*: calculated values.

IV. RESULTS AND DISCUSSION

4.1 Density

Tables 4 shows the Redlich-Kister coefficients and the standard deviation (Eq. 5) between experimental and calculated values of excess molar volume for 1,2- dimethylbenzene + octane, or nonane or decane binary mixtures. A good performance of Redlich-Kister correlations have been obtained and can be observed in Figure 1.

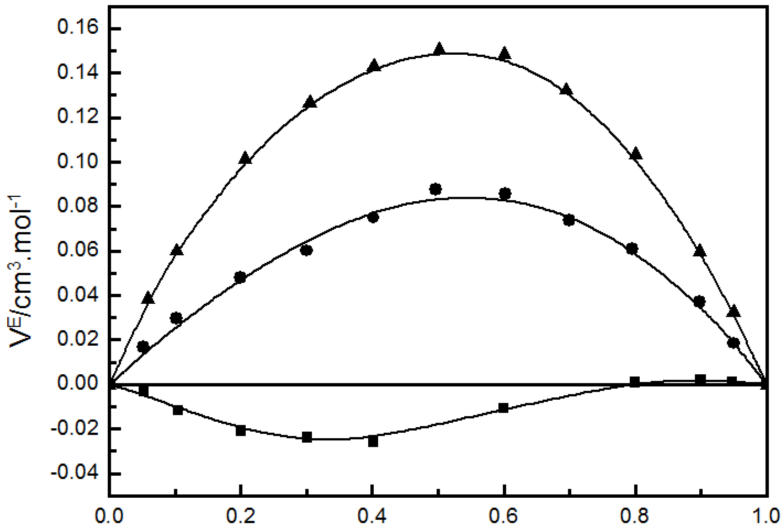
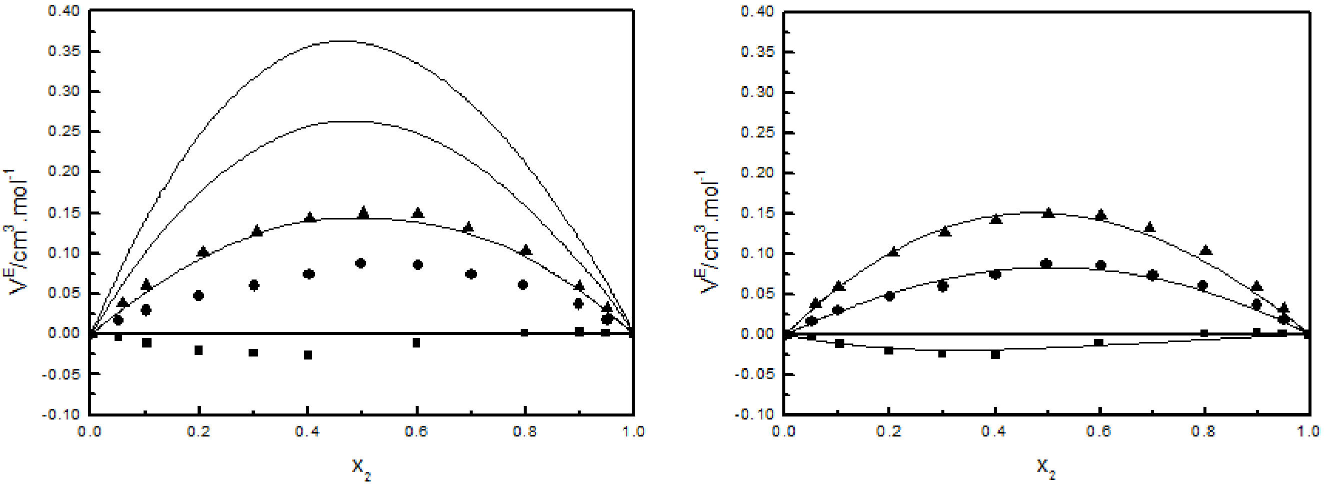


FIGURE 1. EXPERIMENTAL (SYMBOLS) AND REDLICH-KISTER (LINES) CORRELATION FOR THE EXCESS MOLAR VOLUME AT 298.15 FOR 1,2-DIMETHYLBENZENE (1) WITH ALKANES (2) BINARY MIXTURES: OCTANE (■), NONANE(●) AND DECANE(▲).

From Table 2, it can be stated that densities of the alkanes are lower than 1,2-dimethylbenzene, and density of the binaries mixtures increases with an increasing of the length of the alkane. The same behavior is presented for the excess molar volume of these binary mixtures. In Figure 2 it can be observed that 1,2-dimethylbenzene + octane presents an *S*-shaped dependence on composition with small positive values at the highest octane concentration and negative values on the other extreme. However the 1,2-dimethylbenzene + nonane and 1,2-dimethylbenzene + decane binaries mixtures present a maximum excess molar volume at the equimolar composition.



(A) **(B)**

FIGURE 2. COMPARISON BETWEEN EXPERIMENTAL (SYMBOLS) AND MODELING (LINES) EXCESS MOLAR VOLUME FOR 1,2-DIMETHYLBENZENE (1) WITH ALKANES (2) BINARY MIXTURES: OCTANE (■), NONANE (●) OR DECANE (▲) AT 298.15 K. A) NITTA-CHAO PREDICTIONS AND (B) ERAS CORRELATIONS.

Figure 2, also, shows the comparison between experimental excess molar volume data and Nitta–Chao predictions and ERAS correlations of 1,2-dimethylbenzene with octane, nonane and decane at 298.15 K. Tables 5 and 6 shows the parameters used in these modeling, respectively. Significant deviation between experimental results and Nitta-Chao predictions are presented in these binary systems. Also, the Nitta-Chao model cannot recognize the *S* shaped for the mixture of dimethylbenzene with octane. However, the ERAS model is more adequate to model this kind of mixture as it can be observed in Figure 2.b. Very low standard deviation showed in Table 6 has been obtained in the ERAS modeling.

Yang et al.[2] and Gayol et al.[42] have studied the excess molar volume for 1,4-dimethylbenzene + alkanes. From these different studies they have showed an increasing of excess molar volume with the increasing of the alkyl chain length. Yang et al. [2] suggest that this behavior is due to different molecular packings between 1,4-dimethylbenzene + alkane due to the different length chain of the alkanes, because no specific interactions are presented between these kind of molecules. The excess molar volume of 1,2-dimethylbenzene + alkanes, also increases with an increasing of the alkyl chain length. For this situation, similar conclusion can be done for the 1,2-dimethylbenzene + alkane binary mixture studied in this work.

Figure 3 shows a comparison in the excess molar volume for the different isomers of dimethylbenzene with octane at 298.15 K: 1,3-dimethylbenzene [43]; 1,4-dimethylbenzene[2] and 1,2-dimethylbenzene, presented in this work. While the excess molar volume for 1,3-dimethylbenzene and 1,4-dimethylbenzene are positive in all range of compositions, the mixture with 1,2-dimethylbenzene presents a *S* shaped with positive values at octane high compositions. These excess volume values have gone increased for dimethylbenzene isomers + alkane family binary mixtures with the alkane chain length, because all the excess volume are negatives for dimethylbenzene isomers + heptane at 293.15K [44].

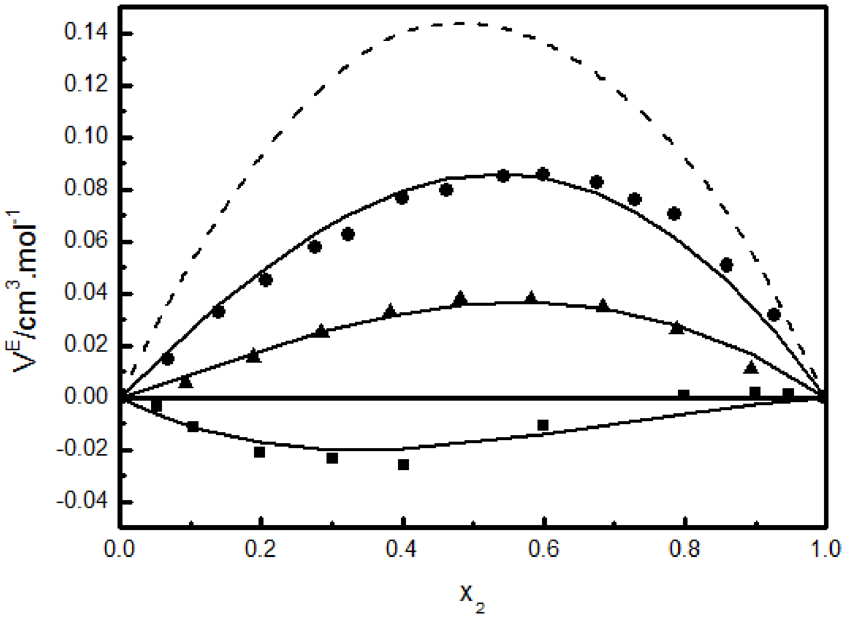


FIGURE 3. EXPERIMENTAL AND MODELING EXCESS MOLAR VOLUME (SYMBOLS) FOR 1,2-DIMETHYLBENZENE (■) (THIS WORK) OR 1,3-DIMETHYLBENZENE (●)[43] OR 1,4-DIMETHYLBENZENE (▲)[2] WITH OCTANE (X2) AT 298.15 K. THE DASH LINE CORRESPONDS TO NITTA-CHAO PREDICTIONS WHILE THE SOLIDS LINES CORRESPOND TO SIMPLIFIED ERAS MODEL CORRELATIONS.

According Figure 3, the excess molar volume follows the order 1,3-dimethylbenzene > 1,4-dimethylbenzene > 1,2-dimethylbenzene with octane at 298.15K. The same order is found for the mixtures of dimethylbenzene isomers with 2-propanol or 2-methyl-2-propanol at 298.15 [26]; acetone or 2-butanone at 298.15 K[25], isopropyl ether or methyl tert-butyl ether at 298.15 K[45] and heptane[44] at 293.15K. As it can be observed in this Figure, the CH_3 positions in the isomers of the dimethylbenzene determine the magnitude of the excess volume [46]. Aromatic hydrocarbons molecules present a large positive quadrupole moment due the accumulation of negative charge in the middle of the ring and positive on the outside which causes an orientational order in these liquids [47]. Furthermore, Figure 3 also include the Nitta-Chao predictions and ERAS correlations for the family of dimethylbenzene with octane at 298.15. As Nitta-Chao model cannot recognize the different isomers, the same line is represented for the three different isomers with octane. The lowest deviation between experimental results and Nitta-Chao predictions are found for the isomer 1,3-dimethylbenzene[43] with octane. However, the ERAS model is capable to reproduce adequately the behavior of the different dimethyl benzene isomers + octane.

4.2 Surface tension results

Surface tension is a consequence of the difference in the molecules distribution between the bulk and the surface of the liquid. The surface tension of alkanes are lower than 1,2-dimethylbenzene, and the deviation surface tension of the binary mixtures increases with the chain length of the alkane because the strength of dispersion forces increases[12] as it can be observed from Figure 4.

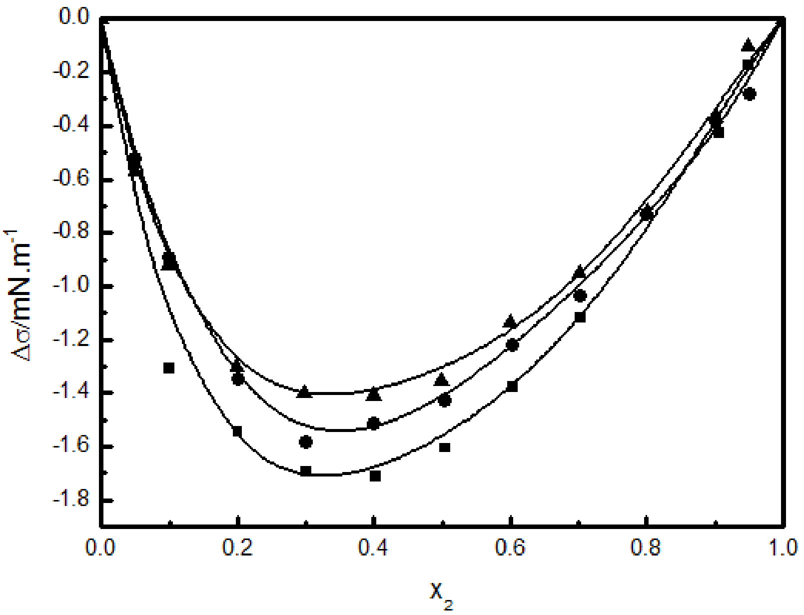


FIGURE 4. EXPERIMENTAL (SYMBOLS) AND REDLICH-KISTER (LINES) CORRELATION FOR THE DEVIATION SURFACE TENSION AT 298.15 K FOR 1,2-DIMETHYLBENZENE (1) WITH ALKANES (2) BINARY MIXTURES: OCTANE (■), NONANE(●) AND DECANE(▲).

Positives surface tension deviation represents chemical effects between the molecules while negatives values are obtained when physical effects and dipolar-dipolar interaction are involved [48]. For the 1,2-dimethylbenzene + alkane binary systems studied in this work, physical effects are more dominant than chemical effects, therefore, they have presented negative values in this property with a minimum in the molar fraction of 1,2-dimethylbenzene near to 0.6-0.7. The same behavior had been found for the 1,4-dimethylbenzene + alkane at 308.15, presented by Gayol et al. [49].

Table 7 and Figure 4 show the Redlich-Kister coefficients, the standard deviation (Eq. 5) and the modeling respectively between experimental and calculated values of surface tension deviation for 1,2- dimethylbenzene + octane, or nonane or decane binary mixtures. Good results have been obtained from this correlation process.

TABLE 7
REDLICH-KISTER COEFFICIENTS AND STANDARD DEVIATIONS S FOR SURFACE TENSION DEVIATION Δσ OBTAINED FOR FITS OF EQ. 4 IN THE INVESTIGATED SYSTEMS AT 298.15 K.

A_0/mN.m^{-1}	A_1/mN.m^{-1}	A_2/mN.m^{-1}	A_3/mN.m^{-1}	$^*SD$/mN.m^{-1}
octane (x_1) + 1,2-Dimethylbenzene (x_2)				
-6.2851	3.0257	-3.3900	3.4023	0.0710
nonane (x_1) + 1,2-Dimethylbenzene (x_2)				
-5.6866	3.2633	-2.5698	-	0.0255
decane (x_1) + 1,2-Dimethylbenzene (x_2)				
-5.2522	2.1986	-2.7781	2.9003	0.0283

Figure 5 explore the surface tension deviation behavior of the different dimethylbenzene isomers with alkanes: 1,2-dimethylbenzene (this work) and 1,4-dimethylbenzene[18] with decane and 1,3-dimethylbenzene with hexane at 298.15 K [37]. The lack of experimental information avoids the comparison between the behaviors of dimethylbenzene isomers with the same hydrocarbon. Negative surface tension deviation for the three binary systems in all range of compositions has been found. For binary systems containing decane, the surface tension deviation of 1,4-dimethylbenzene is higher than the systems containing 1,2-dimethylbenzene. The surface tension deviation is similar for the mixtures containing 1,2-dimethylbenzene and 1,3-dimethylbenzene while a larger surface tension deviation is presented for the mixture containing 1,4-dimethylbenzene. These results are in agreement with those reported by Domínguez-Pérez[24] for the propyl propanoate + dimethylbenzene isomers.

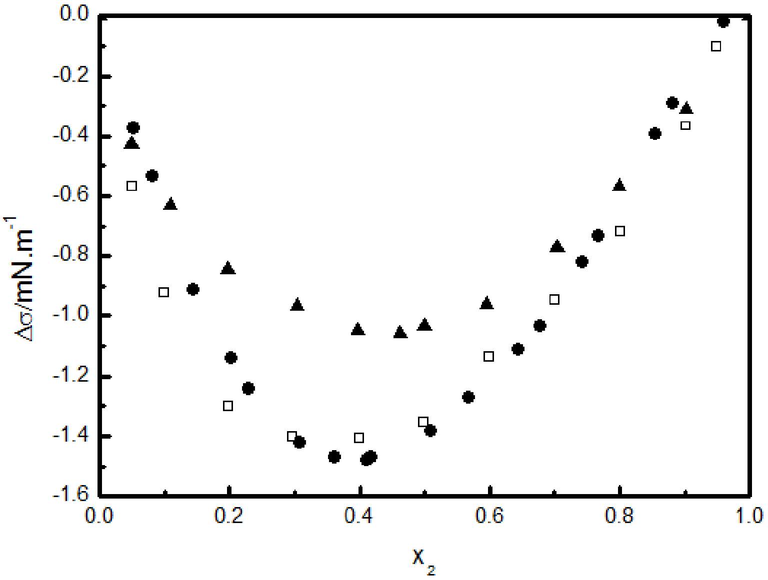


FIGURE 5. EXPERIMENTAL SURFACE TENSION DEVIATION OF DIMETHYLBENZENE ISOMERS (1) + ALKANES (2): 1,2-DIMETHYLBENZENE + DECANE (□) (THIS WORK), 1,4-DIMETHYLBENZENE + DECANE (▲)[18] AND 1,3-DIMETHYLBENZENE + HEXANE AT 298.15K(●) [37].

Figure 6, shows the prediction of the surface tension deviation using the HSIS, HSEG and SE models for 1,2-dimethylbenzene + octane, nonane and decane at 298.15K. Table 8 shows the standard deviation calculated according Equation 5.

TABLE 8
STANDARD DEVIATION OF HSIS, HSEG AND SE MODEL IN THE SURFACE TENSION DEVIATION MODELING OF THE ALKANE (1) + 1,2-DIMETHYLBENZENE (2) BINARY SYSTEM

System	$^{*}SD$/mN.m^{-1}		
	HSIS model	**HSEG model**	**SE model**
octane (x_1) + 1,2-Dimethylbenzene (x_2)	0.69	0.44	0.54
nonane (x_1) + 1,2-Dimethylbenzene (x_2)	0.66	0.39	0.13
decane (x_1) + 1,2-Dimethylbenzene (x_2)	0.68	0.38	0.31

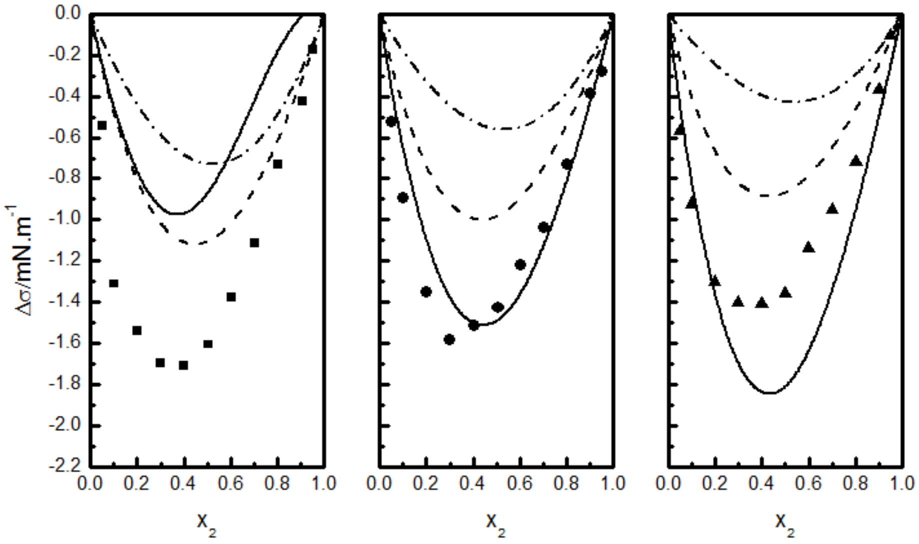


FIGURE 6: COMPARISON BETWEEN EXPERIMENTAL (SYMBOLS) AND MODELING RESULTS (LINES) FOR THE DEVIATION SURFACE TENSION AT 298.15 K IN 1,2-DIMETHYLBENZENE (1) WITH ALKANES (2) BINARY MIXTURES: OCTANE (■), NONANE(●) AND DECANE(▲). THE LINES ARE: SE (—); HSEG (----); HSIS (-.-.-) MODELS.

In general, as it can be observed from this Figure these models reproduce qualitatively their behaviors. A good prediction in the 1-2 dimethyl benzene + nonane has been obtained with the SE model.

V. CONCLUSION

Density and surface tension of 1,2-dimethylbenzene + octane, nonane or decane binary mixtures at 298.15K and atmospheric pressure are presented. Excess molar volume and surface tension deviation have been calculated and correlated by Redlich-Kister polynomial equation. These data allow comparing excess volume molar and surface tension deviation between the different dimethylbenzene isomers + alkane binary mixtures.

No differentiation between the different isomers of dimethylbenzene family is obtained with Nitta-Chao model, while, ERAS model can reproduce correctly all the systems studied in this work. HSIS, HSEG and SE models predict qualitative the surface tension deviation in 1-2 dimethylbenzene + alkanes binary mixtures.

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