J. Chem. Thermodynamics 69 (2014) 193–200

Contents lists available at ScienceDirect

J. Chem. Thermodynamics

journal homepage: www.elsevier.com/locate/jct

Experimental and Nitta–Chao model prediction of high pressure density of *p*-xylene with dialkyl carbonates or *n*-alkanes

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ARTICLE INFO

Article history:
Received 7 July 2013
Received in revised form 26 September 2013
Accepted 27 September 2013
Available online 21 October 2013

Keywords:
Dialkyl carbonate
n-Alkane
p-Xylene
High pressure density

ABSTRACT

New data of high pressure density have been reported for *p*-xylene 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 and they have been compared with those available in the literature. The high pressure density has been correlated and predicted using a modified Tait equation and Nitta Chao group contribution model respectively. The derived thermophysical properties such as isothermal compressibility (κ_T), isobaric thermal expansivity (α_P) and internal pressure (π) have been also calculated.

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1. Introduction

Density is a very important physical property in the chemical and engineering process and influences their operations. The knowledge of this property allows calculating derived thermophysical properties such as isothermal compressibility, isobaric thermal expansivity and internal pressure with a high importance in the industrial process.

Alkanes are employed in different industries as lubricants, fuels, surfactants, polymers, liquid crystals and many biological molecules [1]. Regarding xylenes they are used as raw material in plastic industry to produce synthetic fibers and soft plastic for aircrafts and other vehicles [2]. On the other hand, dialkyl carbonates are present in a high variety of applications in the industrial processes including gasoline additive to reduce emission of pollutants, such as CO, NO_x, unburned hydrocarbons and polynuclear aromatics; also they are used as paint solvents, synthesis of pharmaceuticals and agrochemicals extractive processes, battery technology [3,4]. The mixtures between dialkyl carbonates and aromatics, possess certain properties, for example, miscible with gasoline, stable in storage, and allowable by the emission restriction of the clean air legislation to benefit specific applications [5]. On the other hand, the aromatics and alkanes binary mixtures are present in the crude oil and the knowledge of their behavior is a priority.

The investigation developed in this work continues the study on the thermophyscial properties of pure compounds, binary and ternary mixtures containing dialkyl carbonates, alkanes and alkylbenzenes [6–11] involved in the gasoline field. Particularly, in this work, the high pressure density of *p*-xylene and their binary mixtures with dimethyl carbonate, diethyl carbonate, *n*-octane and *n*-decane has been studied in the (288.15 to 308.15) K temperature range and (0.1 to 40) MPa pressure range.

The available information of dimethyl carbonate, diethyl carbonate, *n*-octane and *n*-decane pure components densities at different temperatures and pressures were studied in a previous work [10]. The available experimental information regarding pure *p*-xylene is presented in many publications in the (288.18 to 598.15) K temperature range and (0.1 to 200) MPa pressure range [5,8,12–26]. However few data are comparable with those reported in this work and they have been gathered in table 1. With the same aim, figure 1 shows the variation in density *vs.* pressure at (288.15, 298.15, 308.15) K and the relative density deviation plot at T = 298.15 K [15,16].

Also table 1 presents the reference of density for *p*-xylene with dimethyl carbonate [22,27], diethyl carbonate [7,22], *n*-octane [23,28,29] and *n*-decane [7,19,26,27,29] binary mixtures at 0.1 MPa. No further information data at high pressure was found for these binary systems.

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http://dx.doi.org/10.1016/j.jct.2013.09.039

TABLE 1
Comparison of the density of *p*-xylene pure component and their binary mixtures between this work and the available literature.

Pure compounds	T/K	$\rho/(g \cdot cm^{-3})$	
		This work	References
		0.1 MPa	
p-Xylene	288.15	0.8649	0.86520 [8]
	298.15	0.8562	0.85651 [20] 0.85658 [8] 0.8565 [24] 0.8597 [16]
	308.15	0.8475	0.8479 [26] 0.84783 [8] 0.84788 [25] 0.8479 [24]

$\rho/(g \cdot cm^{-3})$

T/K	5 MPa	10 MPa		20 MPa		30 MPa		40 MPa	
	This work	This work	Ref.	This work	Ref.	This work	Ref.	This work	Ref.
288.15	0.8683	0.8718		0.8781		0.8840		0.8897	
298.15	0.8602	0.8635	0.8673 [16]	0.8701	0.8736 [16]	0.8765	0.8800 [16]	0.8822	0.8858 [16]
308.15	0.8514	0.8552		0.8621		0.8686		0.8748	

Binary systems		T range/K at 0.1 MPa	References
p-Xylene	Dimethyl carbonate	288.15 to 298.15	[27]
		298.15	[22]
	Diethyl carbonate	288.15 to 308.15	[7]
		298.15	[22]
	n-Octane	293.15	[28]
		298.15	[29]
		298.15 to 353.15	[23]
	n-Decane	288.15 to 298.15	[27]
		288.15 to 308.15	[7]
		298.15	[19,29]
		303.15 to 313.15	[26]

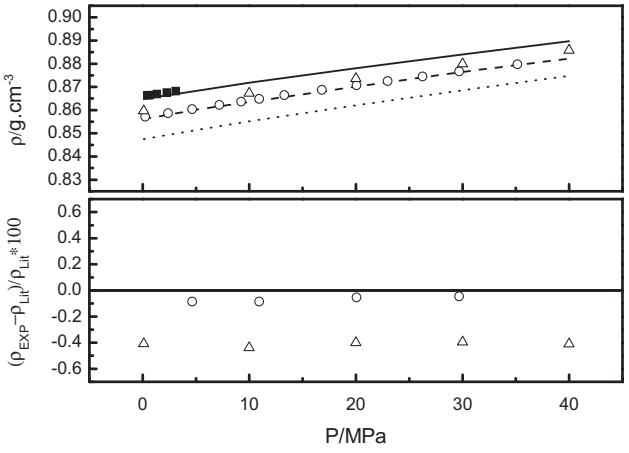


FIGURE 1. High pressure density ρ for pure *p*-xylene against pressure P at different temperature and relative density deviation plot at $T = 298.15$ K. This work: (–) $T = 288.15$ K, (- -) $T = 298.15$ K, (. . .) $T = 308.15$ K. Literature: ■ $T = 288.21$ K [15]; Δ $T = 298.15$ K [16]; o $T = 298.16$ K [15] (smoothed).

2. Experimental section

Table 2, reports the purity, supplier and CAS-number of the compounds used in this work. These products have not had an extra purification.

An analytical balance (AND HM 202) with a precision of $\pm 10^{-4}$ g has been used for all the weighings giving as a result an uncertainty of ±0.0001 in the mole fractions compositions of the mixtures. The components were weighted in volatility decreasing order to avoid losses by evaporation of the components.

A vibrating-tube Anton Paar DMA 4500 densimeter connected to an external Anton Paar 512 P high-pressure measuring cell has been used to determine the densities of pure compounds and binary mixtures. The set provides a density repeatability of 10^{-5} g · cm^{-3} and allowed density measurements up to 70 MPa. A PolyScience 9510 thermostatic bath has been used to achieve the stability temperature which is measured using a CKT-100 platinum probe placed in the measuring cell with an uncertainty lower than $5 \cdot 10^{-2}$ K. A Ruska 7610 pressure controller with a stability of $2 \cdot 10^{-3}$ MPa has been used to generate and control the pressure in the system. A Teflon membrane separator provided by Pressurements has been used to separate the oil used as hydraulic fluid from the sample. The sample pressure has been measured with a SI digital manometer with an uncertainty of 10^{-2} MPa through the separator membrane. Earlier publications [30] explain with more details the experimental technique. Vacuum and water fluids were used for the densimeter calibration according to the procedure of Lagourette *et al.* [31]. This method ensures an uncertainty in density measurement lower than 10^{-4} g · cm^{-3} over wide ranges of pressure and temperature.

According this procedure, density of *p*-xylene pure component and their mixtures with dimethyl carbonate, diethyl carbonate, *n*-octane, *n*-decane have been measured at (288.15, 298.15 and 308.15) K and (0.1, 5, 10, 20, 30 and 40) MPa.

TABLE 2
Purity, supplier and CAS-number of studied compounds.

Compound name	CAS-number	Supplier	[a]Purity (mass fraction)
n-Octane	111-65-9	Sigma Aldrich	⩾0.99
n-Decane	124-18-5	Sigma Aldrich	⩾0.99
Dimethyl carbonate	616-38-6	Fluka	⩾0.99
Diethyl carbonate	105-58-8	Fluka	⩾0.995
p-Xylene	106-42-3	Sigma Aldrich	⩾0.99

[a] No further purification of these products was carried out.

TABLE 3
Nitta–Chao parameters involved in the *p*-xylene + dialkyl carbonates and *p*-xylene + *n*-alkanes binary mixtures. Numbers in bold have been determined in this work.

Group	$V^*_{i,0}/(cm^3 \cdot mol^{-1})$	a_i/K	c_i	Q_i
		Pure group		
$-CH_3$	13.46	23.7	0.338	6.71
$-CH_2$	10.25	23.7	0.093	4.27
–OCOO–	23.48	0.6	0.025	8.86
$-CH_{ar}$	7.98	33.28	0.174	3.13
$-C_{ar-al}$	**4.70**	33.28	-0.127	0.95
		Binary parameters		
i	*j*	$\varepsilon_{ij} = \varepsilon_{ji}/(J \cdot mol^{-1})$	$\sigma^0_{ij} = \sigma^0_{ji}/(J \cdot mol^{-1})$	$\sigma'_{ij} = \sigma'_{ji}/(J \cdot mol^{-1})$
$-CH_3$	$-CH_3$	2515	0	0
	$-CH_2$	2515	0	0
	–OCOO–	2488	0	0
	$-CH_{ar}$	3276	0	0
	$-C_{ar-al}$	3276	0	0
$-CH_2$	$-CH_2$	2515	0	0
	–OCOO–	2488	0	0
	$-CH_{ar}$	3276	0	0
	$-C_{ar-al}$	3276	0	0
–OCOO–	–OCOO–	4648	311	412
	$-CH_{ar}$	**1254**	**0**	**0**
	$-C_{ar-al}$	**1254**	**0**	**0**
$-CH_{ar}$	$-CH_{ar}$	4284	0	0
	$-C_{ar-al}$	4284	0	0
$-C_{ar-al}$	$-C_{ar-al}$	4284	0	0

3. Modified Tait equation

A modified Tait equation [32] has been used to correlate the experimental data of density for each composition of the binary mixtures containing dimethyl carbonate, diethyl carbonate,

TABLE 4
Experimental densities $\rho/g \cdot cm^{-3}$ for dimethyl carbonate (1) + *p*-xylene (2) binary mixtures.

	$\rho/(g \cdot cm^{-3})$					
x_1/P/MPa	0.1	5	10	20	30	40
			T = 288.15 K			
0.0432	0.8718	0.8755	0.8791	0.8854	0.8913	0.8971
0.1950	0.8942	0.8978	0.9013	0.9078	0.9140	0.9201
0.3968	0.9242	0.9319	0.9357	0.9425	0.9490	0.9553
0.4933	0.9449	0.9504	0.9541	0.9614	0.9679	0.9743
0.5296	0.9533	0.9573	0.9612	0.9683	0.9749	0.9809
0.5993	0.9684	0.9724	0.9763	0.9837	0.9905	0.9971
0.7034	0.9923	0.9962	1.0003	1.0078	1.0147	1.0214
0.8023	1.0106	1.0149	1.0190	1.0268	1.0339	1.0407
0.8921	1.0381	1.0425	1.0466	1.0545	1.0615	1.0687
0.9478	1.0529	1.0572	1.0614	1.0694	1.0767	1.0838
			T = 298.15 K			
0.0432	0.8630	0.8673	0.8704	0.8771	0.8834	0.8891
0.1950	0.8845	0.8883	0.8921	0.8992	0.9055	0.9117
0.3968	0.9178	0.9225	0.9258	0.9332	0.9399	0.9465
0.4933	0.9358	0.9406	0.9440	0.9516	0.9587	0.9651
0.5296	0.9425	0.9471	0.9507	0.9582	0.9654	0.9720
0.5993	0.9573	0.9620	0.9657	0.9734	0.9805	0.9873
0.7034	0.9805	0.9854	0.9891	0.9970	1.0044	1.0112
0.8023	0.9984	1.0034	1.0073	1.0155	1.0227	1.0301
0.8921	1.0255	1.0306	1.0347	1.0429	1.0506	1.0579
0.9478	1.0400	1.0449	1.0490	1.0575	1.0650	1.0727
			T = 308.15 K			
0.0432	0.8543	0.8581	0.8620	0.8691	0.8757	0.8817
0.1950	0.8752	0.8793	0.8833	0.8907	0.8975	0.9040
0.3968	0.9076	0.9121	0.9162	0.9240	0.9312	0.9379
0.4933	0.9252	0.9297	0.9341	0.9418	0.9494	0.9563
0.5296	0.9317	0.9362	0.9404	0.9484	0.9560	0.9630
0.5993	0.9463	0.9508	0.9552	0.9583	0.9709	0.9781
0.7034	0.9690	0.9737	0.9782	0.9864	0.9942	1.0015
0.8023	0.9864	0.9910	0.9956	1.0044	1.0122	1.0198
0.8921	1.0131	1.0180	1.0227	1.0315	1.0397	1.0474
0.9478	1.0272	1.0321	1.0368	1.0457	1.0540	1.0617

TABLE 5
Experimental densities $\rho/g \cdot cm^{-3}$ for diethyl carbonate (1) + *p*-xylene (2) binary mixtures.

	$\rho/(g \cdot cm^{-3})$					
x_1/P/MPa	0.1	5	10	20	30	40
			T = 288.15 K			
0.1014	0.8767	0.8801	0.8837	0.8903	0.8961	0.9021
0.1346	0.8795	0.8841	0.8878	0.8943	0.9003	0.9063
0.1949	0.8875	0.8912	0.8948	0.9013	0.9075	0.9134
0.2767	0.8983	0.9009	0.9045	0.9113	0.9174	0.9235
0.3860	0.9092	0.9134	0.9172	0.9241	0.9304	0.9366
0.4858	0.9207	0.9247	0.9285	0.9355	0.9419	0.9483
0.5444	0.9284	0.9315	0.9353	0.9425	0.9491	0.9554
0.5923	0.9339	0.9370	0.9410	0.9480	0.9547	0.9612
0.6718	0.9423	0.9464	0.9503	0.9575	0.9643	0.9709
0.7676	0.9532	0.9574	0.9613	0.9687	0.9756	0.9823
0.8313	0.9606	0.9648	0.9689	0.9764	0.9833	0.9901
0.9044	0.9687	0.9731	0.9772	0.9847	0.9919	0.9986
			T = 298.15 K			
0.1014	0.8676	0.8719	0.8751	0.8820	0.8882	0.8943
0.1346	0.8715	0.8758	0.8790	0.8859	0.8923	0.8984
0.1949	0.8781	0.8824	0.8858	0.8927	0.8993	0.9053
0.2767	0.8875	0.8920	0.8954	0.9025	0.9091	0.9153
0.3860	0.8998	0.9044	0.9077	0.9150	0.9219	0.9282
0.4858	0.9107	0.9152	0.9188	0.9263	0.9332	0.9396
0.5444	0.9168	0.9220	0.9256	0.9332	0.9402	0.9466
0.5923	0.9228	0.9274	0.9311	0.9385	0.9458	0.9523
0.6718	0.9317	0.9365	0.9403	0.9478	0.9551	0.9618
0.7676	0.9424	0.9473	0.9510	0.9590	0.9663	0.9731
0.8313	0.9498	0.9547	0.9584	0.9664	0.9738	0.9808
0.9044	0.9576	0.9627	0.9666	0.9747	0.9822	0.9891
			T = 308.15 K			
0.1014	0.8587	0.8628	0.8666	0.8738	0.8804	0.8866
0.1346	0.8625	0.8667	0.8704	0.8777	0.8845	0.8908
0.1949	0.8689	0.8730	0.8765	0.8842	0.8911	0.8975
0.2767	0.8782	0.8824	0.8865	0.8938	0.9008	0.9073
0.3860	0.8901	0.8945	0.8985	0.9062	0.9133	0.9199
0.4858	0.9007	0.9052	0.9092	0.9172	0.9245	0.9312
0.5444	0.9072	0.9117	0.9160	0.9239	0.9313	0.9381
0.5923	0.9126	0.9169	0.9214	0.9294	0.9368	0.9437
0.6718	0.9213	0.9257	0.9303	0.9384	0.9459	0.9529
0.7676	0.9318	0.9365	0.9409	0.9492	0.9570	0.9641
0.8313	0.9390	0.9436	0.9481	0.9566	0.9642	0.9716
0.9044	0.9467	0.9515	0.9562	0.9645	0.9726	0.9799

TABLE 6
Experimental densities ρ/g · cm^{-3} for *n*-octane (1) + *p*-xylene (2) binary mixtures.

	ρ/(g · cm^{-3})					
x_1/P/MPa	0.1	5	10	20	30	40
			T = 288.15 K			
0.0509	0.8549	0.8583	0.8618	0.8683	0.8742	0.8800
0.0993	0.8451	0.8490	0.8525	0.8588	0.8648	0.8706
0.1981	0.8264	0.8302	0.8337	0.8404	0.8464	0.8522
0.2961	0.8088	0.8126	0.8162	0.8229	0.8290	0.8349
0.3989	0.7914	0.7952	0.7989	0.8056	0.8119	0.8178
0.4891	0.7766	0.7808	0.7846	0.7913	0.7978	0.8038
0.5473	0.7683	0.7720	0.7757	0.7827	0.7891	0.7951
0.6039	0.7601	0.7635	0.7672	0.7742	0.7805	0.7865
0.8031	0.7459	0.7496	0.7533	0.7603	0.7663	0.7727
0.8963	0.7197	0.7238	0.7275	0.7348	0.7411	0.7472
0.9460	0.7127	0.7167	0.7208	0.7276	0.7342	0.7403
			T = 298.15 K			
0.0509	0.8461	0.8504	0.8534	0.8603	0.8663	0.8725
0.0993	0.8365	0.8408	0.8440	0.8507	0.8571	0.8631
0.1981	0.8179	0.8223	0.8255	0.8324	0.8389	0.8449
0.2961	0.8002	0.8046	0.8080	0.8150	0.8215	0.8275
0.3989	0.7829	0.7874	0.7909	0.7980	0.8045	0.8107
0.4891	0.7687	0.7733	0.7766	0.7840	0.7907	0.7968
0.5473	0.7607	0.7644	0.7680	0.7752	0.7819	0.7879
0.6039	0.7521	0.7559	0.7595	0.7668	0.7733	0.7794
0.8031	0.7373	0.7420	0.7455	0.7530	0.7597	0.7659
0.8963	0.7122	0.7165	0.7200	0.7273	0.7341	0.7405
0.9460	0.7047	0.7095	0.7132	0.7207	0.7275	0.7338
			T = 308.15 K			
0.0509	0.8374	0.8414	0.8452	0.8521	0.8589	0.8650
0.0993	0.8280	0.8320	0.8358	0.8429	0.8496	0.8558
0.1981	0.8093	0.8135	0.8175	0.8245	0.8314	0.8377
0.2961	0.7916	0.7960	0.8000	0.8073	0.8142	0.8205
0.3989	0.7744	0.7788	0.7830	0.7903	0.7972	0.8037
0.4891	0.7603	0.7647	0.7689	0.7764	0.7834	0.7897
0.5473	0.7524	0.7559	0.7601	0.7677	0.7746	0.7812
0.6039	0.7439	0.7472	0.7516	0.7593	0.7663	0.7727
0.8031	0.7291	0.7337	0.7378	0.7455	0.7527	0.7592
0.8963	0.7042	0.7081	0.7124	0.7201	0.7274	0.7340
0.9460	0.6975	0.7013	0.7055	0.7134	0.7207	0.7273

TABLE 7
Experimental densities ρ/g · cm^{-3} for *n*-decane (1) + *p*-xylene (2) binary mixtures.

	ρ/(g · cm^{-3})					
x_1/P/MPa	0.1	5	10	20	30	40
			T = 288.15 K			
0.0513	0.8540	0.8580	0.8614	0.8679	0.8738	0.8795
0.0971	0.8453	0.8494	0.8528	0.8592	0.8650	0.8708
0.1962	0.8282	0.8316	0.8350	0.8415	0.8474	0.8533
0.2932	0.8121	0.8159	0.8194	0.8257	0.8318	0.8376
0.3942	0.7998	0.8035	0.8069	0.8135	0.8194	0.8251
0.4987	0.7841	0.7877	0.7914	0.7977	0.8038	0.8094
0.5563	0.7772	0.7807	0.7842	0.7908	0.7967	0.8025
0.5965	0.7739	0.7770	0.7795	0.7860	0.7920	0.7981
0.7018	0.7610	0.7647	0.7684	0.7748	0.7807	0.7863
0.8047	0.7508	0.7544	0.7579	0.7643	0.7704	0.7760
0.8975	0.7410	0.7451	0.7486	0.7556	0.7619	0.7681
0.9474	0.7380	0.7418	0.7452	0.7515	0.7576	0.7632
			T = 298.15 K			
0.0513	0.8457	0.8501	0.8533	0.8600	0.8662	0.8721
0.0971	0.8371	0.8413	0.8444	0.8512	0.8576	0.8634
0.1962	0.8196	0.8237	0.8270	0.8338	0.8402	0.8460
0.2932	0.8040	0.8082	0.8114	0.8184	0.8247	0.8304
0.3942	0.7916	0.7958	0.7992	0.8060	0.8124	0.8182
0.4987	0.7760	0.7805	0.7836	0.7904	0.7968	0.8026
0.5563	0.7690	0.7734	0.7767	0.7836	0.7899	0.7957
0.5965	0.7650	0.7687	0.7719	0.7788	0.7852	0.7911
0.7018	0.7532	0.7576	0.7608	0.7677	0.7740	0.7798
0.8047	0.7429	0.7472	0.7505	0.7574	0.7637	0.7695
0.8975	0.7346	0.7386	0.7418	0.7482	0.7552	0.7616
0.9474	0.7304	0.7346	0.7380	0.7447	0.7509	0.7572
			T = 308.15 K			
0.0513	0.8372	0.8413	0.8449	0.8519	0.8588	0.8651
0.0971	0.8286	0.8326	0.8365	0.8434	0.8498	0.8560
0.1962	0.8111	0.8152	0.8191	0.8260	0.8327	0.8389
0.2932	0.7957	0.7999	0.8037	0.8106	0.8174	0.8236
0.3942	0.7835	0.7877	0.7914	0.7986	0.8052	0.8113
0.4987	0.7681	0.7721	0.7761	0.7833	0.7899	0.7959
0.5563	0.7610	0.7652	0.7693	0.7764	0.7830	0.7891
0.5965	0.7570	0.7606	0.7645	0.7717	0.7782	0.7850
0.7018	0.7463	0.7496	0.7535	0.7606	0.7670	0.7733
0.8047	0.7361	0.7394	0.7433	0.7503	0.7570	0.7631
0.8975	0.7279	0.7313	0.7348	0.7419	0.7485	0.7551
0.9474	0.7232	0.7268	0.7309	0.7379	0.7444	0.7509

n-octane and *n*-decane with *p*-xylene in all range of temperature and pressure according to the following expression:

$$\rho(P,T) = \frac{\rho(P_0,T)}{1 - C\ln\left(\frac{B(T)+P}{B(T)+P_0}\right)}, \quad (1)$$

where P_0 is the reference pressure of 0.1 MPa and C is a temperature independent parameter. In this case of study the best fit of the reference pressure densities $\rho(P_0,T)$ was found with a polynomial of grade one:

$$\rho(P_0,T) = \rho_{00} + \rho_{01}T \quad (2)$$

and $B(T)$ with a polynomial of grade two:

$$B(T) = B_0 + B_1T + B_2T^2, \quad (3)$$

where ρ_{00}, ρ_{01}, B_0, B_1, B_2 are the fitting parameters.

SigmaPlot Software has been used to determine the adjustable parameters of the modified Tait equation using *Dynamic Fit Wizard* option with a Marquardt–Levenberg.

The thermomechanical coefficients of isothermal compressibility (κ_T), isobaric thermal expansivity (α_P) and internal pressure (π) can be derived from the equation (1) and they are presented in a previous work [10].

4. Nitta–Chao modeling

The high pressure density of dialkyl carbonates or *n*-alkanes with *p*-xylene binary mixtures have been predicted by a group contribution model called Nitta–Chao [33]. This model is able to predict the vaporization enthalpy, PVT relations and molar volume for polar and non polar liquids and the Gibbs free energy, excess enthalpies, excess volume, heat capacities, activity coefficients and the existence of a chemical association term for their solutions.

The cell theory with the repulsive forces between molecules derived from Carnahan–Starling equation of state [34] for hard spheres is the base for the Nitta–Chao model.

Dialkyl carbonates, *n*-alkanes and *p*-xylene were described by the molecular groups carbonate (–OCOO–), methyl (–CH_3), methylene (–CH_2), aromatic ring CH (CH_{ar}) and aromatic ring C bonded to a side chain (C_{ar-al}) groups following the procedure of García *et al.* [35] and Eckart *et al.* [36].

Each group contribution *i* is defined by the hard core volume V_i^*, its temperature dependence coefficient a_i, the number of external degrees of freedom c_i and the number of contact of the groups Q_i calculated according to Bondi [37]. The energetic interactions parameters between the group *i* with the group *j* are: the dispersive parameters ε_{ij}, the non-dispersive parameters σ_{ij}^0 representing the dipole–dipole interaction between groups and its temperature dependence coefficient σ_{ij}'. Previous works [33,38] explain with more details the model. The pure parameters and the interaction parameters between carbonate, methyl and methylene were taken from Lugo *et al.* [39] and those for the aromatic ring and aromatic ring C bonded to a side chain were taken from Eckart *et al.* [36]. In this work, the hard core volume for the C_{ar-al} group has been recalculated and the interaction parameters between CH_{ar} and

TABLE 8
Modified Tait equation coefficients for the dialkyl carbonates + *p*-xylene and *n*-alkanes + *p*-xylene binary mixtures.

x_1	ρ_{00}/g · cm^{-3}	ρ_{01}/g · cm^{-3} · K^{-1}	C	B_0/MPa	B_1/MPa · K^{-1}	B_2/MPa · K^{-2}	AAD[a]/g · cm^{-3}	APD[a]/%
Dimethyl carbonate (1) + p-xylene (2)								
0.0000	1.1163	$-8.7226 \cdot 10^{-4}$	0.0801	896.20	−4.7956	$7.0 \cdot 10^{-3}$	$1.1 \cdot 10^{-4}$	$1.3 \cdot 10^{-2}$
0.0432	1.1250	$-8.7864 \cdot 10^{-4}$	0.0713	−200.89	2.3467	$-4.7 \cdot 10^{-3}$	$4.0 \cdot 10^{-4}$	$4.5 \cdot 10^{-2}$
0.1950	1.1685	$-9.5223 \cdot 10^{-4}$	0.0832	−246.58	3.0056	$-6.3 \cdot 10^{-3}$	$4.5 \cdot 10^{-4}$	$4.9 \cdot 10^{-2}$
0.3968	1.1628	$-8.2581 \cdot 10^{-4}$	0.0449	−151.42	1.1277	$-1.6 \cdot 10^{-3}$	$1.1 \cdot 10^{-3}$	$1.2 \cdot 10^{-1}$
0.4933	1.2291	$-9.8541 \cdot 10^{-4}$	0.0614	56.263	0.2549	$-8.0 \cdot 10^{-4}$	$3.0 \cdot 10^{-4}$	$3.2 \cdot 10^{-2}$
0.5296	1.2648	$-1.0809 \cdot 10^{-3}$	0.0796	606.96	−2.7881	$3.5 \cdot 10^{-3}$	$1.4 \cdot 10^{-4}$	$1.5 \cdot 10^{-2}$
0.5993	1.2872	$-1.1064 \cdot 10^{-3}$	0.1891	4089.5	−24.892	$4.0 \cdot 10^{-2}$	$6.2 \cdot 10^{-4}$	$6.4 \cdot 10^{-2}$
0.7034	1.3275	$-1.1636 \cdot 10^{-3}$	0.0803	146.25	0.2820	$-1.6 \cdot 10^{-3}$	$2.0 \cdot 10^{-4}$	$2.0 \cdot 10^{-2}$
0.8023	1.3592	$-1.2098 \cdot 10^{-3}$	0.0817	67.517	0.7579	$-2.3 \cdot 10^{-3}$	$2.3 \cdot 10^{-4}$	$2.2 \cdot 10^{-2}$
0.8921	1.3985	$-1.2508 \cdot 10^{-3}$	0.0817	541.34	−2.3370	$2.7 \cdot 10^{-3}$	$5.5 \cdot 10^{-4}$	$5.2 \cdot 10^{-2}$
0.9478	1.4228	$-1.2839 \cdot 10^{-3}$	0.0849	211.13	−0.0824	$-1.1 \cdot 10^{-3}$	$6.0 \cdot 10^{-4}$	$5.7 \cdot 10^{-2}$
Diethyl carbonate (1) + p-xylene (2)								
0.1014	1.1351	$-8.9686 \cdot 10^{-4}$	0.0763	400.74	−1.5577	$1.7 \cdot 10^{-3}$	$4.9 \cdot 10^{-4}$	$5.5 \cdot 10^{-2}$
0.1346	1.1234	$-8.4589 \cdot 10^{-4}$	0.0646	−178.17	1.8773	$-3.5 \cdot 10^{-3}$	$6.4 \cdot 10^{-4}$	$7.1 \cdot 10^{-2}$
0.1949	1.1551	$-9.2867 \cdot 10^{-4}$	0.0836	423.26	−1.6010	$1.6 \cdot 10^{-3}$	$5.4 \cdot 10^{-4}$	$6.0 \cdot 10^{-2}$
0.2767	1.1883	$-1.0072 \cdot 10^{-3}$	0.0911	993.99	−4.8901	$6.4 \cdot 10^{-3}$	$3.6 \cdot 10^{-4}$	$4.0 \cdot 10^{-2}$
0.3860	1.1846	$-9.5549 \cdot 10^{-4}$	0.0731	199.99	−0.3690	$-2.0 \cdot 10^{-4}$	$7.1 \cdot 10^{-4}$	$7.7 \cdot 10^{-2}$
0.4858	1.2102	$-1.0047 \cdot 10^{-3}$	0.0768	320.57	−1.0025	$7.0 \cdot 10^{-4}$	$4.6 \cdot 10^{-4}$	$4.9 \cdot 10^{-2}$
0.5444	1.2330	$-1.0581 \cdot 10^{-3}$	0.0789	636.78	−2.8934	$3.5 \cdot 10^{-3}$	$3.9 \cdot 10^{-4}$	$4.1 \cdot 10^{-2}$
0.5923	1.2404	$-1.0642 \cdot 10^{-3}$	0.0894	527.17	−1.9681	$1.8 \cdot 10^{-3}$	$4.3 \cdot 10^{-4}$	$4.6 \cdot 10^{-2}$
0.6718	1.2437	$-1.0464 \cdot 10^{-3}$	0.078	359.82	−1.2851	$1.2 \cdot 10^{-3}$	$3.7 \cdot 10^{-4}$	$3.9 \cdot 10^{-2}$
0.7676	1.2610	$-1.0685 \cdot 10^{-3}$	0.0787	539.40	−2.4686	$3.1 \cdot 10^{-3}$	$3.4 \cdot 10^{-4}$	$3.5 \cdot 10^{-2}$
0.8313	1.2726	$-1.0825 \cdot 10^{-3}$	0.0825	603.69	−2.8509	$3.7 \cdot 10^{-3}$	$4.5 \cdot 10^{-4}$	$4.7 \cdot 10^{-2}$
0.9044	1.2854	$-1.0991 \cdot 10^{-3}$	0.0762	451.16	−1.9305	$2.3 \cdot 10^{-3}$	$5.4 \cdot 10^{-4}$	$5.5 \cdot 10^{-2}$
n-Octane (1) + p-xylene (2)								
0.0509	1.1063	$-8.7257 \cdot 10^{-4}$	0.0802	296.90	−0.8170	$4.0 \cdot 10^{-4}$	$1.9 \cdot 10^{-4}$	$2.2 \cdot 10^{-2}$
0.0993	1.0924	$-8.5824 \cdot 10^{-4}$	0.0760	−42.778	1.3299	$-3.1 \cdot 10^{-3}$	$3.2 \cdot 10^{-4}$	$3.8 \cdot 10^{-2}$
0.1981	1.0726	$-8.5427 \cdot 10^{-4}$	0.0749	454.36	−2.0451	$2.6 \cdot 10^{-3}$	$1.6 \cdot 10^{-4}$	$1.9 \cdot 10^{-2}$
0.2961	1.0560	$-8.5787 \cdot 10^{-4}$	0.0741	156.61	−0.0494	$-8.0 \cdot 10^{-4}$	$1.1 \cdot 10^{-4}$	$1.3 \cdot 10^{-2}$
0.3989	1.0361	$-8.4928 \cdot 10^{-4}$	0.0753	571.32	−2.8503	$3.9 \cdot 10^{-3}$	$1.8 \cdot 10^{-4}$	$2.3 \cdot 10^{-2}$
0.4891	1.0106	$-8.1193 \cdot 10^{-4}$	0.0739	598.17	−3.1953	$4.7 \cdot 10^{-3}$	$3.2 \cdot 10^{-4}$	$4.1 \cdot 10^{-2}$
0.5473	0.9976	$-7.9553 \cdot 10^{-4}$	0.1109	171.31	0.0895	$-1.0 \cdot 10^{-3}$	$2.8 \cdot 10^{-4}$	$3.6 \cdot 10^{-2}$
0.6039	0.9931	$-8.0846 \cdot 10^{-4}$	0.1171	113.90	0.6588	$-2.2 \cdot 10^{-3}$	$2.1 \cdot 10^{-4}$	$2.8 \cdot 10^{-2}$
0.8031	0.9878	$-8.3962 \cdot 10^{-4}$	0.0809	737.71	−3.8816	$5.5 \cdot 10^{-3}$	$2.1 \cdot 10^{-4}$	$2.8 \cdot 10^{-2}$
0.8963	0.9433	$-7.7561 \cdot 10^{-4}$	0.0995	186.08	−0.2153	$-4.0 \cdot 10^{-4}$	$3.2 \cdot 10^{-4}$	$4.3 \cdot 10^{-2}$
0.9460	0.9321	$-7.6196 \cdot 10^{-4}$	0.0908	490.15	−2.4070	$3.4 \cdot 10^{-3}$	$2.8 \cdot 10^{-4}$	$4.0 \cdot 10^{-2}$
n-Decane (1) + p-xylene (2)								
0.0513	1.0962	$-8.4051 \cdot 10^{-4}$	0.0717	79.600	0.4177	$-1.4 \cdot 10^{-3}$	$5.8 \cdot 10^{-4}$	$6.7 \cdot 10^{-2}$
0.0971	1.0863	$-8.3621 \cdot 10^{-4}$	0.0684	351.05	−1.5088	$1.9 \cdot 10^{-3}$	$2.0 \cdot 10^{-4}$	$2.4 \cdot 10^{-2}$
0.1962	1.0737	$-8.5219 \cdot 10^{-4}$	0.0810	642.41	−3.1061	$4.1 \cdot 10^{-3}$	$5.5 \cdot 10^{-4}$	$6.6 \cdot 10^{-2}$
0.2932	1.0482	$-8.1941 \cdot 10^{-4}$	0.0754	444.64	−1.9864	$2.5 \cdot 10^{-3}$	$1.7 \cdot 10^{-4}$	$2.1 \cdot 10^{-2}$
0.3942	1.0352	$-8.1682 \cdot 10^{-4}$	0.0739	457.96	−2.0747	$2.6 \cdot 10^{-3}$	$2.9 \cdot 10^{-4}$	$3.6 \cdot 10^{-2}$
0.4987	1.0157	$-8.0374 \cdot 10^{-4}$	0.0743	397.95	−1.6811	$2.0 \cdot 10^{-3}$	$5.1 \cdot 10^{-4}$	$6.5 \cdot 10^{-2}$
0.5563	1.0097	$-8.0717 \cdot 10^{-4}$	0.0730	558.77	−2.7600	$3.7 \cdot 10^{-3}$	$6.2 \cdot 10^{-4}$	$7.8 \cdot 10^{-2}$
0.5965	1.0181	$-8.4802 \cdot 10^{-4}$	0.1555	440.68	−0.1410	$-2.6 \cdot 10^{-3}$	$2.4 \cdot 10^{-4}$	$3.1 \cdot 10^{-2}$
0.7018	0.9728	$-7.3541 \cdot 10^{-4}$	0.0856	358.26	−1.5232	$2.0 \cdot 10^{-3}$	$2.2 \cdot 10^{-4}$	$2.9 \cdot 10^{-2}$
0.8047	0.9619	$-7.3329 \cdot 10^{-4}$	0.0934	332.53	−1.2140	$1.3 \cdot 10^{-3}$	$5.7 \cdot 10^{-4}$	$7.5 \cdot 10^{-2}$
0.8975	0.9307	$-6.5810 \cdot 10^{-4}$	0.1336	−461.83	4.0161	$-6.8 \cdot 10^{-3}$	$2.0 \cdot 10^{-4}$	$2.7 \cdot 10^{-2}$
0.9474	0.9513	$-7.4041 \cdot 10^{-4}$	0.0930	581.70	−2.7936	$3.8 \cdot 10^{-3}$	$1.6 \cdot 10^{-4}$	$2.1 \cdot 10^{-2}$

[a] AAD : $\frac{1}{N}\sum_{i=1}^{N}|\rho_i^{exp} - \rho_i^{cal}|$; APD = $\frac{100}{N}\sum_{i=1}^{N}\left|\frac{\rho_i^{exp}-\rho_i^{cal}}{\rho_i^{exp}}\right|$ where N is the number of experimental data, exp: experimental data and cal: calculated values.

C_{ar-al} with –OCOO– have been obtained using the Marquardt's non-linear regression procedure algorithm [40] with constraints imposed by the physical significance of the parameters [41]. All parameters are showed in table 3 and the number in bold are the parameters obtained in this work. As it can be seen from this table, the interactions energies between polar groups have dispersive and non-dispersive parameters, whereas the interactions between the polar groups and aliphatic groups are only dispersive.

5. Results and discussion

High pressure density for the dimethyl carbonate + *p*-xylene; diethyl carbonate + *p*-xylene; *n*-octane + *p*-xylene and *n*-decane + *p*-xylene binary mixtures have been measured in this work and they are presented in tables 4–7.

Table 8 presents the coefficients for the modified Tait equation (equation (1)) beside the average absolute deviation (AAD) and average percentual deviation (APD) for each composition in all range of temperature and pressure studied. The parameters of dimethyl carbonate, diethyl carbonate, *n*-octane and *n*-decane pure component have been reported in a previous work [10].

Figure 1 shows the pure *p*-xylene density at (288.15, 298.15, 308.15) K and the relative density deviations between the data reported in this work and those comparable experimental data available in the literature at T = 298.15 K [15,16] against pressure. The relative density deviation range is (−0.4 to 0)% and they are lower for the data presented by Castro *et al.* [15] than Yokoyama *et al.* [16].

Figure 2 presents the comparison between the experimental high pressure density with Tait correlation at (288.15 to 308.15) K for dimethyl carbonate + *p*-xylene; *n*-octane + *p*-xylene; binary systems in a fixed molar compositions. The densities of the dimethyl carbonate + *p*-xylene and *n*-decane + *p*-xylene are higher than the diethyl carbonate + *p*-xylene and the *n*-octane + *p*-xylene respectively; a decreasing of density with

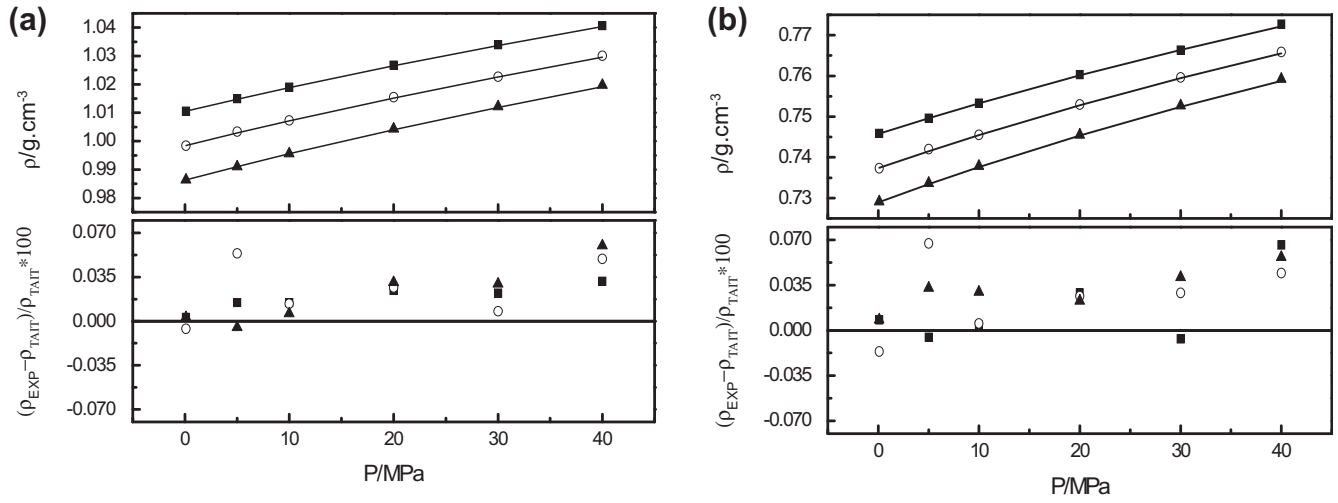


FIGURE 2. Comparison between experimental (symbols) with Tait correlation (lines) of high pressure binary mixtures density ρ and relative density deviation plot at fixed compositions against pressure P of: (a) dimethyl carbonate (1) + p-xylene (2) (x_1 = 0.8023); (b) n-octane (1) + p-xylene (2) (x_1 = 0.8031). The temperatures are: ■ T = 288.15 K, ○ T = 298.15 K, ▲ T = 308.15 K.

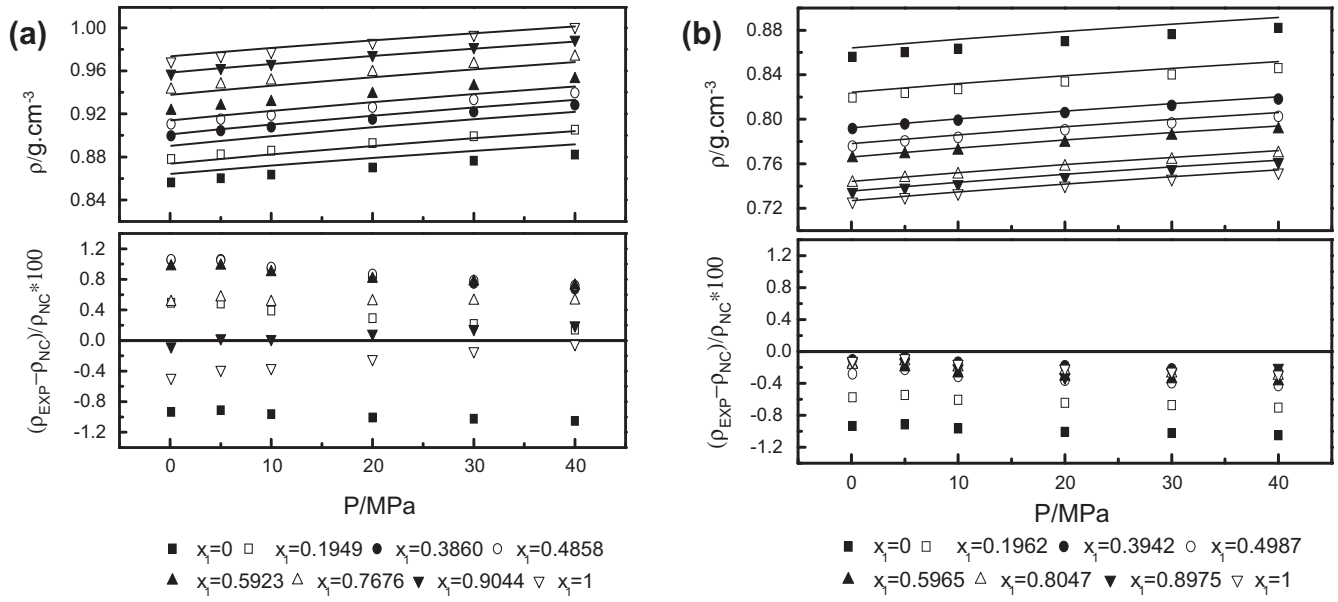


FIGURE 3. High pressure density ρ and relative density deviation plot of binary mixtures containing p-xylene against pressure P at T = 298.15 K for: (a) diethyl carbonate (1) + p-xylene (2), (b) n-decane + p-xylene (2) at different compositions. Experimental data: symbols. Nitta–Chao predictions: lines.

temperature and good correlations using the modified Tait equation in all systems studied. From the combined figure 2, it can be observed relative density deviations between the experimental values and Tait correlations of (0.07 to −0.02)% for the dimethyl carbonate (1) + p-xylene (2) at x_1 = 0.8023 and n-octane (1) + p-xylene at x_1 = 0.8031 binary mixtures.

The different volumetric behavior between dimethyl carbonate + p-xylene and diethyl carbonate + p-xylene is due to the formation of $n-\pi$ complexes between the free electrons of the carbonate group and the aromatic ring [22].

Regarding n-alkanes + p-xylene, there is no specific interactions between both molecules, however, the behavior of n-octane + p-xylene and n-decane + p-xylene may be related to the different molecular packing due to the different molecular chain lengths of the alkanes [23] and in this case, the density of n-alkanes + p-xylene increases with the increasing length of the alkane.

Figure 3 shows the comparison between the experimental and the Nitta–Chao prediction in the high pressure density of the diethyl carbonate + p-xylene (a) and n-decane + p-xylene (b) binary mixtures at different fixed compositions at T = 298.15 K. Nitta–Chao model predict adequately the behavior of the high pressure density for all systems studied.

The relative density deviations between the experimental values and Nitta–Chao predictions presented in figure 3 are (1 to −1)% at T = 298.15 K in diethyl carbonate + p-xylene and n-decane + p-xylene binary mixtures. Pure p-xylene presents the high deviations between the experimental and Nitta–Chao predictions.

The mean APD for all binary systems studied in overall range compositions were (0.04 and 1.06)% using the Tait equation correlation and Nitta–Chao prediction respectively. The high deviations have found in the dimethyl carbonate + p-xylene binary mixtures

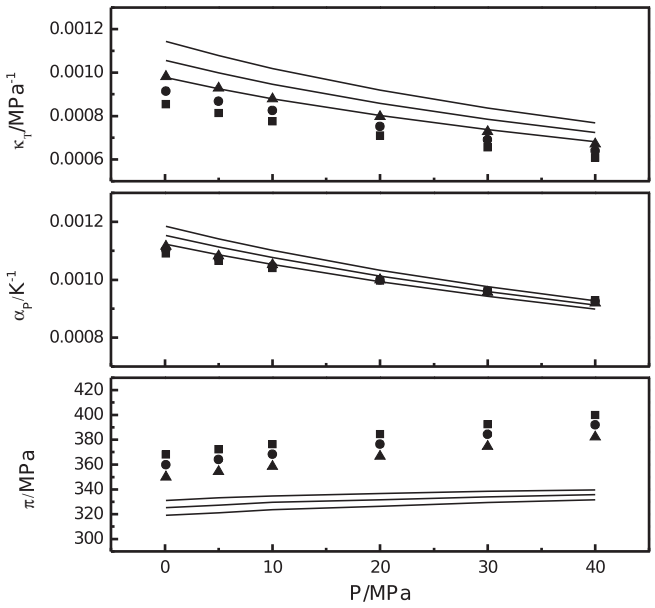


FIGURE 4. Comparison between experimental data (symbols) and Nitta–Chao prediction (lines) for the isothermal compressibility (κ_T), isobaric thermal expansivity (α_P) and internal pressure (π) against pressure P for diethyl carbonate (1) + p-xylene (2) system at $x_1 = 0.4858$. The temperatures are: ■ $T = 288.15$ K, ● $T = 298.15$ K, ▲ $T = 308.15$ K.

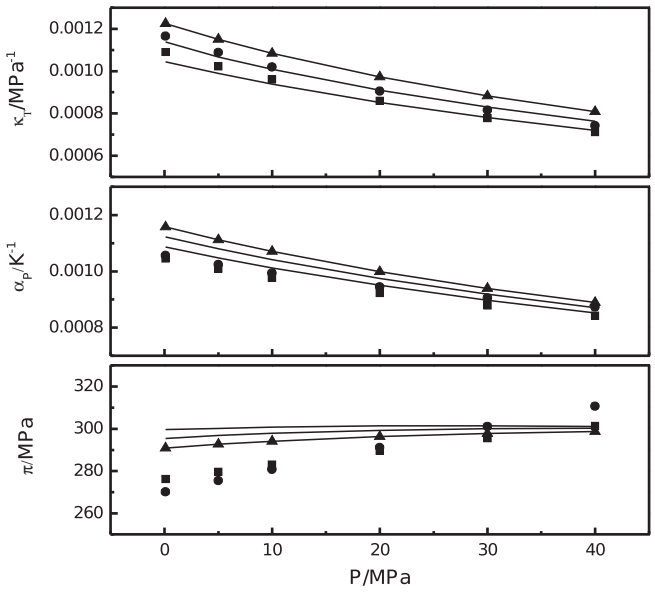


FIGURE 5. Comparison between experimental data (symbols) and Nitta–Chao prediction (lines) for the isothermal compressibility (κ_T), isobaric thermal expansivity (α_P) and internal pressure (π) against pressure P for n-octane (1) + p-xylene (2) system at $x_1 = 0.4891$. The temperatures are: ■ $T = 288.15$ K, ● $T = 298.15$ K, ▲ $T = 308.15$ K.

with a maximum APD of (0.12 and 2.57)% for Tait equation correlation and Nitta–Chao prediction, respectively.

Figures 4 and 5 show the experimental and predicted Nitta–Chao isothermal compressibility (κ_T), isobaric thermal expansivity (α_P) and internal pressure (π) for a fixed molar compositions of diethyl carbonate + p-xylene and n-octane + p-xylene respectively at (288.15, 298.15 and 308.15) K. As a previous work [10], Nitta–Chao predictions shows a low accurate in the internal pressure as it can be seen from figures 4 and 5; however the deviation remains small. The mean APD between the experimental and predicted Nitta–Chao model showed in figure 4, for the isothermal compressibility (κ_T), isobaric thermal expansivity (α_P) and internal pressure (π) of diethyl carbonate + p-xylene are (2.7; 14.4; 11.5)%, respectively. The same deviation in these properties for the n-octane + p-xylene showed in figure 5 are (3.6; 2.1 and 5.1)%, respectively.

As it can be seen from figures 4 and 5, the isothermal compressibility (κ_T) and the isobaric thermal expansivity (α_P) increases with the temperature and decreases with the pressure whereas the internal pressure decreases with the temperature and increases with the pressure. This tendency is general for the remaining compositions of dimethyl carbonate + p-xylene and n-decane + p-xylene and the diethyl carbonate + p-xylene and n-octane + p-xylene.

The values of isothermal compressibility, isobaric thermal expansivity and internal pressure for dimethyl carbonate + p-xylene and n-octane + p-xylene are bigger than in diethyl carbonate + p-xylene and n-decane + p-xylene, respectively, due to the insertion of methylene groups.

6. Conclusion

New high pressure densities are presented in this work for p-xylene + dimethyl carbonate, p-xylene + diethyl carbonate, p-xylene + n-octane, p-xylene + n-decane. The value of this work is the increasing of the available information examined in this work, because the only data accessible at this moment from our knowledge is at 0.1 MPa for all systems studied. The experimental density data have been correlated and predicted with Tait and Nitta–Chao model, respectively. Also the derived properties such as isothermal compressibility, isobaric thermal expansivity and internal pressure have been also explored.

Acknowledgments

The authors are grateful to Universidad de Vigo and Ministerio de Educación y Ciencia from Spain (Projects FIS2011-23322 and CGL2008-03668), and CONICET, Universidad Nacional de Córdoba and Universidad Tecnológica Nacional from Argentine for financial support.

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