Volumetric properties of (dialkyl carbonate + *n*-alkane) mixtures at high pressures: Experimental measurement and Nitta–Chao model prediction

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ABSTRACT

The present work reports valuable experimental high-pressure density data for dimethyl carbonate, diethyl carbonate, *n*-octane, *n*-decane pure components and their binary mixtures (dialkyl carbonate + *n*-alkane) at temperatures between (288.15 and 308.15) K and pressures between (0.1 and 40) MPa. The experimental density values were compared with experimental information available in the literature. While the volumetric properties for (dimethyl carbonate + *n*-alkane) were reported in many works, the (diethyl carbonate + *n*-alkane) were less studied. The purpose of this study is to extend the available experimental information about the thermophysical behavior of this kind of mixtures, which is useful in the fuel field. The experimental density data were correlated using a modified Tait equation and were predicted by Nitta–Chao group contribution model.

1. Introduction

In the last years, organic carbonates as dimethyl and diethyl carbonates have been considered as replacement of traditional oxygenated gasoline additive such as methyl tertiary butyl ether. This compound, widely used as gasoline additive for octane and oxygen enhancement, was found to be polluting groundwater, it is not biodegradable and it is a potential human carcinogen [1]. On the other hand, dialkyl carbonates are non-toxic and environmentally friendly products capable to reduce pollutant emissions as carbon monoxide, nitrogen oxides, hydrocarbons and particulate matter [2]. They have high oxygen content, which makes them an outstanding oxygenate, have good blending octane and they do not phase separate in a water stream [3]. Furthermore, these kinds of molecules as dimethyl carbonate and diethyl carbonate have been proposed as lubricants of the new refrigerants, hydrofluorocarbons and as paint solvents [4].

Moreover, gasoline is a mixture of C_4 to C_{12} hydrocarbons, including aliphatic and aromatic hydrocarbons. Consequently, the study of volumetric properties of (dialkylcarbonate + *n*-alkane) mixtures is important to analyze the use of dimethyl carbonate

and diethyl carbonate as fuel additive. For this reason, several authors have studied this kind of systems in recent years. The available information about volumetric properties of dimethyl carbonate [5–7], diethyl carbonate [7], *n*-octane [5,8–10], and *n*-decane [6,8] pure component and (dialkyl carbonate + *n*-alkane) binary systems, are summarized in table 1 including the reference, temperature, and pressure range. As can be observed, the volumetric properties of pure components were studied in a wide range of temperature and pressure as well as for (dimethyl carbonate + *n*-octane) [5,11,12] and (dimethyl carbonate + *n*-decane) systems [6,12]. However, the volumetric properties for diethyl carbonate with these alkanes are scarce and it is only available at atmospheric pressure from our knowledge [13,14]. In this way, this work studies the density of dimethyl carbonate, diethyl carbonate, *n*-octane, *n*-decane pure component, and (dialkyl carbonate + *n*-alkane) binary mixtures in a broader range of temperature {from (288.15 to 318.15) K} and pressure {from (0.1 to 40) MPa}.

A modified Tait equation [15] was used to fit the density values and to obtain the derived properties such as isothermal compressibility coefficient (κ_T), isobaric thermal expansivity coefficient (α_P) and internal pressure (π). Also, the ability of the Nitta–Chao [16] model for the prediction of density values and derived properties was determined in this work for all systems studied.

2. Experimental

2.1. Materials

n-Octane (⩾0.99 mass fraction) and *n*-decane (⩾0.99 mass fraction) were supplied by Sigma Aldrich, while dimethyl carbonate

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TABLE 1
References of pure compounds and binary mixtures density found in the literature.

Pure compounds		T range/K	P range/MPa	Ref.
Dimethyl carbonate		278.15 to 353.15	0.1 to 25	Lugo et al. [5]
		283.15 to 328.15	0.1 to 40	Troncoso et al. [6]
		283.15 to 353.15	0.1 to 60	Comuñas et al. [7]
Diethyl carbonate		283.15 to 353.15	0.1 to 60	Comuñas et al. [7]
n-Octane		278.15 to 353.15	0.1 to 25	Lugo et al. [5]
		298.03 to 348.14	0.1 to 35.2	Dymond et al. [8]
		303.15 to 393.15	0 to 117.6	Boelhouwer [9]
		258.00 to 333.15	0.1 to 28	Benson and Winnick [10]
n-Decane		283.15 to 328.15	0.1 to 40	Troncoso et al. [6]
		298.31 to 373.10	0.1 to 500.1	Dymond et al. [8]
		Binary systems		
n-Octane	Dimethyl carbonate	288.15 to 308.15	0.1	Pardo et al. [11]
		293.15 to 318.15	0.1	Tojo et al. [12]
		278.15 to 353.15	0.1 to 25	Lugo et al. [5]
	Diethyl carbonate	293.15 to 313.15	0.1	Rodriguez et al. [13]
n-Decane	Dimethyl carbonate	298.15 to 318.15	0.1	Tojo et al. [12]
		288.15 to 328.15	0.1 to 40	Troncoso et al. [6]
	Diethyl carbonate	288.15 to 308.15	0.1	Mosteiro et al. [14]

TABLE 2
Group characteristic parameters used in application of the Nitta–Chao model for (dialkyl carbonate + n-alkane).

Group	$V_{i,0}^*/(cm^3 \cdot mol^{-1})$			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	
–OCOO–	23.48			0.6			0.025	8.86	
	$\varepsilon_{ij}/(J \cdot mol^{-1})$			$\sigma_{ij}^0/(J \cdot mol^{-1})$			$\sigma_{ij}^t/(J \cdot mol^{-1})$		
	–CH$_3$	–CH$_2$	–OCOO–	–CH$_3$	–CH$_2$	–OCOO–	–CH$_3$	–CH$_2$	–OCOO–
–CH$_3$	2515	2515	2488	0	0	0	0	0	0
–CH$_2$	2515	2515	2488	0	0	0	0	0	0
–OCOO–	2488	2488	4648	0	0	311	0	0	412

(⩾99.0 mass%) and diethyl carbonate (⩾99.5 mass%) were supplied by Fluka. All products were degassed in an ultrasound bath, stored over molecular sieves to remove moisture traces, and kept in inert argon atmosphere. No further purification of these products was carried out.

2.2. Experimental apparatus and procedure

All weighing was carried out in a (AND HM 202) balance with an uncertainty of ±10^{-4} g. The uncertainty in the mole fractions of the prepared mixtures was estimated to be ±0.0001.

Densities of pure compounds and binary mixtures were measured with a vibrating-tube Anton Paar DMA 4500 densimeter, which provides a density repeatability of 10^{-5} g · cm^{-3}, connected to an external Anton Paar 512 P high-pressure measuring cell, which enables density measurements up to 70 MPa. Temperature stability is achieved through a PolyScience 9510 circulating fluid thermostatic bath and temperature is measured using a CKT-100 platinum probe placed by the measuring cell, which ensures an uncertainty lower that 5 · 10^{-2} K. Pressure is generated and controlled using a Ruska 7610 pressure controller, which assures a pressure stability of 2 · 10^{-3} MPa. Oil used as hydraulic fluid is separated from the sample using a Teflon membrane separator provided by Pressurements. A right pressure transmission through the separator membrane is ensured by measuring the sample pressure with a SI digital manometer, with an uncertainty of 10^{-2} MPa. More details about the experimental technique can be found in earlier publications [17]. The densimeter calibration was performed according to the procedure of Lagourette et al. [18] using vacuum and water as calibrating fluids. This method enables obtaining a correct calibration over wide ranges of pressure and temperature and ensures an uncertainty in density determination lower than 10^{-4} g · cm^{-3}. Using this procedure, density of pure dimethyl carbonate, diethyl carbonate, n-octane, n-decane and the binary mixtures between dialkyl carbonate with n-alkanes were measured at (288.15, 298.15, and 308.15) K and (0.1, 5, 10, 20, 30, and 40) MPa.

3. Modified Tait equation

Experimental density values for dimethyl carbonate, diethyl carbonate, n-octane, n-decane pure components, and (dialkyl carbonate + n-alkane) binary mixtures were correlated by modified Tait equation [15]. This equation allows correlate liquid density measurements as a function of temperature and pressure according to the follow expression:

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

where P_0 stands for the reference pressure (0.1 MPa). Reference pressure densities were fitted using a temperature dependent polynomial.

$$\rho(P_0,T) = \sum_{i=0}^{n} \rho_{0i}T^i, \qquad (2)$$

TABLE 3
Experimental densities $\rho/(g \cdot cm^{-3})$ of pure components.

| | | $\rho/(g \cdot cm^{-3})$ | | | | | | | | | | | |
| | P/MPa | 0.1 | | 5 | | 10 | | 20 | | 30 | | 40 | |
	T/K	This work	Literature [6]	This work	Literature [6]	This work	Literature [6]	This work	Literature [6]	This work	Literature [6]	This work	Literature[6]
Dimethyl carbonate	288.15	1.0765	1.0764	1.0806	1.0808	1.0848	1.0850	1.0928	1.0930	1.1003	1.1005	1.1075	1.1075
	298.15	1.0629	1.0631	1.0680	1.0677	1.0721	1.0722	1.0805	1.0807	1.0885	1.0886	1.0959	1.0960
	308.15	1.0496	1.0497	1.0546	1.0546	1.0594	1.0594	1.0683	1.0684	1.0767	1.0768	1.0845	1.0846
		This work	Literature[7]	This work	Literature[7]	This work	Literature[7]	This work	Literature[7]	This work	Literature[7]	This work	Literature[7]
Diethyl carbonate	288.15	0.9803	0.9861[a]	0.9845	0.9901[a]	0.9886	0.9942[a]	0.9963	1.0017[a]	1.0036	1.0087[a]	1.0105	1.0154[a]
	298.15	0.9689	0.9747[b]	0.9738	0.9792[b]	0.9778	0.9834[b]	0.9860	0.9914[b]	0.9936	0.9988[b]	1.0008	1.0058[b]
	308.15	0.9577	0.9634[c]	0.9624	0.9680[c]	0.9671	0.9726[c]	0.9757	0.9811[c]	0.9838	0.9890[c]	0.9913	0.9962[c]
		This work	Literature[5]	This work	Literature[5]	This work	Literature [5]	This work	Literature [5]	This work		This work	
n-Octane	288.15	0.7066	0.7107[a]	0.7109	0.7146[a]	0.7147[a]	0.7183[a]	0.7217	0.7252[a]	0.7281		0.7343	
	298.15	0.6986	0.7027[b]	0.7034	0.7068[b]	0.7070	0.7107[b]	0.7146	0.7180[b]	0.7214		0.7277	
	308.15	0.6905	0.6945[c]	0.6950	0.6989[c]	0.6994	0.7031[c]	0.7073	0.7109[c]	0.7145		0.7208	
		This work	Literature [6]	This work	Literature [6]	This work	Literature [6]	This work	Literature [6]	This work	Literature [6]	This work	Literature[6]
n-Decane	288.15	0.7336	0.7337	0.7372	0.7408	0.7407	0.7406	0.7472	0.7471	0.7532	0.7532	0.7589	0.7589
	298.15	0.7260	0.7262	0.7302	0.7299	0.7335	0.7335	0.7403	0.7404	0.7465	0.7467	0.7522	0.7527
	308.15	0.7183	0.7187	0.7224	0.7225	0.7262	0.7264	0.7334	0.7336	0.7400	0.7401	0.7459	0.7463

[a] Data at 283.15 K.
[b] Data at 293.15 K.
[c] Data at 303.15 K.

where ρ_{0i} is the fitting parameters and n is the order temperature dependent. According the three isotherms studied in this work, the best fit was achieved with a linear equation, so $n = 1$.

In equation (1) C is a temperature independent parameter and $B(T)$ is a polynomial of the form

$$B(T) = \sum_{i=0}^{2} B_i T^i, \qquad (3)$$

where B_i are the fitting parameters.

The evaluation of the adjustable parameters of the Tait function was obtained by the D*ynamic Fit Wizard* option, available in the *SigmaPlot Software*. It uses the Marquardt–Levenberg algorithm to find the parameters of the independent variables that give the best fit between the equation and the experimental data. This algorithm seeks the values of the parameters that minimize the sum of the squared differences between the values of the observed and predicted values of the dependent variable through an iterative process.

From this equation also can be determined the thermomechanical coefficients: isothermal compressibility (κ_T), isobaric thermal expansivity (α_P), and internal pressure (π).

Thus, the expression for each coefficient was derived from equation (1):

$$k_T \equiv -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right) = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial P}\right)_T = \frac{C}{(B(T)+P)\left(1 - C\ln\left(\frac{B(T)+P}{B(T)+P_0}\right)\right)}, \qquad (4)$$

$$\alpha_P \equiv \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P = \frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_P$$
$$= -\frac{d\rho_0/dT}{\rho_0(T)} - \frac{C(P_0-P)dB/dT}{(B(T)+P_0)(B(T)+P)\left(1 - C\ln\left(\frac{B(T)+P}{B(T)+P_0}\right)\right)}, \qquad (5)$$

$$\pi \equiv \left(\frac{\partial U}{\partial v}\right)_T = T\left(\frac{\partial P}{\partial T}\right)_V - P = T\frac{\alpha_P}{k_T} - P. \qquad (6)$$

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

| x_1 | $\rho/(g \cdot cm^{-3})$ P/MPa | | | | | |
	0.1	5	10	20	30	40
			$T = 288.15 K$			
0.0535	0.7164	0.7198	0.7236	0.7309	0.7375	0.7437
0.0978	0.7238	0.7279	0.7319	0.7393	0.7458	0.7520
0.3935	0.7916	0.7969	0.8011	0.8088	0.8160	0.8228
0.4960	0.8229	0.8275	0.8318	0.8396	0.8469	0.8538
0.5475	0.8409	0.8446	0.8490	0.8570	0.8643	0.8712
0.5937	0.8549	0.8620	0.8662	0.8743	0.8816	0.8887
0.7002	0.8996	0.9046	0.9089	0.9170	0.9244	0.9316
0.8013	0.9417	0.9524	0.9569	0.9650	0.9725	0.9797
0.8979	1.0050	1.0090	1.0133	1.0217	1.0291	1.0363
0.9502	1.0368	1.0432	1.0475	1.0557	1.0631	1.0704
			$T = 298.15 K$			
0.0535	0.7074	0.7122	0.7159	0.7236	0.7305	0.7368
0.0978	0.7153	0.7202	0.7241	0.7317	0.7387	0.7451
0.3935	0.7826	0.7878	0.7918	0.8001	0.8077	0.8146
0.4960	0.8126	0.8179	0.8220	0.8304	0.8381	0.8451
0.5475	0.8295	0.8349	0.8390	0.8475	0.8553	0.8625
0.5937	0.8465	0.8517	0.8561	0.8646	0.8724	0.8796
0.7002	0.8886	0.8939	0.8981	0.9068	0.9148	0.9220
0.8013	0.9360	0.9414	0.9456	0.9542	0.9621	0.9697
0.8979	0.9921	0.9973	1.0015	1.0101	1.0180	1.0256
0.9502	1.0259	1.0311	1.0353	1.0437	1.0517	1.0591
			$T = 308.15 K$			
0.0535	0.6992	0.7040	0.7083	0.7163	0.7237	0.7304
0.0978	0.7069	0.7118	0.7162	0.7243	0.7316	0.7384
0.3935	0.7729	0.7781	0.7828	0.7915	0.7996	0.8069
0.4960	0.8023	0.8076	0.8124	0.8213	0.8295	0.8369
0.5475	0.8190	0.8242	0.8291	0.8381	0.8464	0.8539
0.5937	0.8357	0.8410	0.8459	0.8549	0.8633	0.8708
0.7002	0.8773	0.8826	0.8875	0.8966	0.9050	0.9128
0.8013	0.9241	0.9292	0.9344	0.9434	0.9519	0.9597
0.8979	0.9796	0.9846	0.9896	0.9987	1.0071	1.0150
0.9502	1.0131	1.0181	1.0231	1.0321	1.0404	1.0483

TABLE 5
Experimental densities $\rho/\text{g} \cdot \text{cm}^{-3}$ for (dimethyl carbonate (1) + n-decane (2)) binary mixture.

x_1	$\rho/(\text{g} \cdot \text{cm}^{-3})$ P/MPa					
	0.1	5	10	20	30	40
			$T = 288.15\ K$			
0.0438	0.7390	0.7427	0.7462	0.7527	0.7588	0.7643
0.1100	0.7490	0.7536	0.7572	0.7639	0.7698	0.7758
0.2348	0.7692	0.7731	0.7768	0.7837	0.7900	0.7961
0.3516	0.7920	0.7960	0.7999	0.8070	0.8134	0.8197
0.3944	0.8019	0.8059	0.8098	0.8170	0.8235	0.8293
0.5570	0.8445	0.8487	0.8526	0.8588	0.8650	0.8726
0.8035	0.9444	0.9488	0.9531	0.9631	0.9712	0.9778
0.9500	1.0342	1.0385	1.0428	1.0508	1.0582	1.0653
			$T = 298.15\ K$			
0.0438	0.7313	0.7356	0.7390	0.7459	0.7522	0.7581
0.1100	0.7419	0.7462	0.7497	0.7566	0.7631	0.7690
0.2348	0.7608	0.7655	0.7690	0.7762	0.7829	0.7890
0.3516	0.7832	0.7879	0.7914	0.7990	0.8059	0.8122
0.3944	0.7933	0.7980	0.8018	0.8094	0.8166	0.8230
0.5570	0.8314	0.8367	0.8405	0.8483	0.8561	0.8632
0.8035	0.9321	0.9376	0.9421	0.9511	0.9592	0.9668
0.9500	1.0214	1.0265	1.0307	1.0390	1.0470	1.0544
			$T = 308.15\ K$			
0.0438	0.7236	0.7277	0.7317	0.7390	0.7456	0.7518
0.1100	0.7339	0.7382	0.7422	0.7497	0.7564	0.7626
0.2348	0.7525	0.7569	0.7610	0.7686	0.7756	0.7821
0.3516	0.7743	0.7789	0.7832	0.7909	0.7983	0.8049
0.3944	0.7838	0.7885	0.7928	0.8011	0.8084	0.8153
0.5570	0.8202	0.8256	0.8308	0.8400	0.8484	0.8561
0.8035	0.9207	0.9263	0.9316	0.9411	0.9497	0.9578
0.9500	1.0088	1.0138	1.0185	1.0276	1.0359	1.0437

TABLE 6
Experimental densities $\rho/\text{g} \cdot \text{cm}^{-3}$ for (diethyl carbonate (1) + n-octane (2)) binary mixtures.

x_1	$\rho/(\text{g} \cdot \text{cm}^{-3})$ P/MPa					
	0.1	5	10	20	30	40
			$T = 288.15\ K$			
0.0522	0.7160	0.7201	0.7239	0.7312	0.7378	0.7440
0.1042	0.7261	0.7304	0.7344	0.7416	0.7482	0.7545
0.1671	0.7386	0.7428	0.7468	0.7541	0.7607	0.7672
0.3220	0.7726	0.7781	0.7821	0.7896	0.7965	0.8031
0.3657	0.7840	0.7884	0.7926	0.8001	0.8071	0.8137
0.5075	0.8205	0.8249	0.8290	0.8368	0.8439	0.8505
0.6922	0.8742	0.8794	0.8837	0.8916	0.8985	0.9076
0.8002	0.9085	0.9128	0.9170	0.9250	0.9321	0.9390
0.9206	0.9510	0.9549	0.9588	0.9665	0.9738	0.9807
0.9459	0.9598	0.9643	0.9686	0.9763	0.9833	0.9903
			$T = 298.15\ K$			
0.0522	0.7077	0.7125	0.7163	0.7239	0.7308	0.7372
0.1042	0.7177	0.7225	0.7263	0.7340	0.7410	0.7474
0.1671	0.7299	0.7347	0.7385	0.7463	0.7534	0.7599
0.3220	0.7645	0.7695	0.7734	0.7814	0.7888	0.7955
0.3657	0.7747	0.7797	0.7837	0.7918	0.7991	0.8059
0.5075	0.8107	0.8158	0.8198	0.8281	0.8356	0.8424
0.6922	0.8647	0.8698	0.8738	0.8820	0.8898	0.8969
0.8002	0.8977	0.9028	0.9069	0.9152	0.9228	0.9299
0.9206	0.9392	0.9442	0.9482	0.9564	0.9640	0.9711
0.9459	0.9493	0.9538	0.9577	0.9659	0.9736	0.9807
			$T = 308.15\ K$			
0.0522	0.6996	0.7042	0.7087	0.7166	0.7238	0.7305
0.1042	0.7093	0.7140	0.7185	0.7265	0.7339	0.7407
0.1671	0.7212	0.7259	0.7305	0.7387	0.7462	0.7530
0.3220	0.7554	0.7604	0.7651	0.7733	0.7811	0.7880
0.3657	0.7654	0.7704	0.7751	0.7836	0.7912	0.7983
0.5075	0.8010	0.8059	0.8108	0.8194	0.8272	0.8346
0.6922	0.8543	0.8593	0.8641	0.8730	0.8809	0.8883
0.8002	0.8871	0.8920	0.8968	0.9056	0.9137	0.9212
0.9206	0.9280	0.9329	0.9376	0.9463	0.9543	0.9619
0.9459	0.9376	0.9426	0.9473	0.9560	0.9641	0.9715

TABLE 7
Experimental densities $\rho/(\text{g} \cdot \text{cm}^{-3})$ for (diethyl carbonate (1) + n-decane (2)) binary mixture.

x_1	$\rho/(\text{g} \cdot \text{cm}^{-3})$ P/MPa					
	0.1	5	10	20	30	40
			$T = 288.15\ K$			
0.0538	0.7408	0.7445	0.7480	0.7546	0.7606	0.7664
0.1716	0.7594	0.7633	0.7668	0.7736	0.7809	0.7856
0.2151	0.7663	0.7702	0.7737	0.7805	0.7869	0.7928
0.3257	0.7865	0.7905	0.7943	0.8012	0.8075	0.8138
0.5032	0.8213	0.8267	0.8307	0.8378	0.8446	0.8509
0.5482	0.8322	0.8366	0.8406	0.8478	0.8545	0.8609
0.7985	0.9032	0.9074	0.9115	0.9190	0.9260	0.9328
0.8989	0.9375	0.9436	0.9477	0.9554	0.9626	0.9695
0.9487	0.9569	0.9630	0.9671	0.9748	0.9819	0.9889
			$T = 298.15\ K$			
0.0538	0.7331	0.7376	0.7407	0.7477	0.7539	0.7598
0.1716	0.7512	0.7558	0.7591	0.7662	0.7726	0.7787
0.2151	0.7580	0.7626	0.7660	0.7731	0.7798	0.7858
0.3257	0.7779	0.7826	0.7861	0.7935	0.8002	0.8065
0.5032	0.8135	0.8182	0.8219	0.8297	0.8367	0.8433
0.5482	0.8231	0.8278	0.8317	0.8394	0.8465	0.8531
0.7985	0.8928	0.8977	0.9015	0.9096	0.9171	0.9241
0.8989	0.9283	0.9335	0.9375	0.9457	0.9532	0.9602
0.9487	0.9476	0.9527	0.9566	0.9648	0.9722	0.9793
			$T = 308.15\ K$			
0.0538	0.7255	0.7296	0.7336	0.7407	0.7475	0.7536
0.1716	0.7432	0.7475	0.7516	0.7589	0.7658	0.7721
0.2151	0.7499	0.7543	0.7584	0.7659	0.7727	0.7791
0.3257	0.7694	0.7739	0.7781	0.7859	0.7929	0.7994
0.5032	0.8044	0.8090	0.8135	0.8214	0.8289	0.8358
0.5482	0.8139	0.8184	0.8230	0.8310	0.8384	0.8453
0.7985	0.8825	0.8873	0.8920	0.9005	0.9082	0.9156
0.8989	0.9177	0.9226	0.9271	0.9357	0.9438	0.9512
0.9487	0.9366	0.9415	0.9462	0.9546	0.9627	0.9702

4. Nitta-Chao model predictions

Nitta–Chao [16] group contribution model is based on the cell theory with the repulsive forces between molecules being expressed by a modified cell partition function derived from Carnahan–Starling equation of state [19] for hard spheres. Its validity is restricted to high densities. The advantages of this model with respect to other group contribution methods are its greater theoretical rigor, its capacity to predict a large number of thermodynamic properties such as enthalpy of vaporization, PVT relations, excess properties and activity coefficients and the existence of a chemical association term.

Dialkyl carbonates and n-alkanes were described by the molecular groups carbonate (–OCOO–), methyl (–CH$_3$) and methylene (–CH$_2$) groups following the procedure of García et al. [20]. The energetic parameters involving the methylene group are considered to be the same as those of the methyl group as is usually done for other group contribution models.

The structural parameters for the group i are: the hard core volume $V_{i,0}^*$, its temperature dependence coefficient a_i and the number of external degrees of freedom c_i. The number of contact of the groups, Q_i was calculated according to Bondi [21]. The energetic parameters ε_{ij} are the dispersive ones corresponding to the interaction of this group i with the group j, whereas the non-dispersive parameters are σ_{ij}^0, which represents the dipole–dipole interaction between them and its temperature dependence coefficient σ_{ij}'. More details about the Nitta–Chao model can be found in earlier publications [16,22]. These parameters were taken from Lugo et al. [23] and are showed in table 2. The interactions between the aliphatic groups and the polar groups are only dispersive, whereas the interaction energies between polar groups have both, dispersive and non-dispersive, parameters [16].

5. Results and discussion

Density of pure dimethyl carbonate, diethyl carbonate, n-octane, and n-decane were measured at (288.15, 298.15, and 308.15) K and between (0.1 and 40) MPa. The same conditions of temperature and pressure were used in the determination of the experimental density of the four binary systems studied in this work: (dimethyl carbonate + n-octane), (dimethyl carbonate + n-decane), (diethyl carbonate + n-octane), and (diethyl carbonate + n-decane). Tables 3 to 7 report the volumetric properties of pure compounds and binary mixtures while table 8 presents the Tait equation coefficient according equation (1) together with average absolute deviation (AAD) and average percentual deviation (APD). The volumetric properties of pure component reported in table 3, are compared with the information available in the literature at the same conditions of temperature and pressure studied in this work (except for the diethyl carbonate and n-octane where the density are compared at the nearest temperature and the same pressure). The experimental data reported in this work has an APD equal to 0.0307% regarding the available information.

Figure 1 shows experimental and Tait correlations density values against pressure for (dimethyl carbonate + n-octane), (diethyl carbonate + n-octane), (dimethyl carbonate + n-decane), and (diethyl carbonate + n-decane) at different temperatures for an approximately similar fixed composition. The system containing (dialkyl carbonate + n-decane) present higher density with respect at the corresponding (dialkyl carbonate + n-octane) because the dispersive interactions between n-decane molecules are higher than those of n-octane due to its longer alkyl chain. These results are in agreement with Pardo et al. [11] in the study of density for (dimethyl carbonate + n-octane and n-nonane) binary mixtures. Also, as dimethyl carbonate and n-decane present higher density values than diethyl carbonate and n-octane, respectively, the (dimethyl carbonate + n-decane) binary mixture presents the highest density values respect the remaining binary systems studied. From this figure it can be seen a decrease of density with temperature, also observed for all systems studied. Good correlations have been obtained with the modified Tait equation. Available experimental data reported in the literature were added into this figure to compare them with the experimental data of this work [5,6,11–14]. A good agreement was obtained.

Figure 2 shows the experimental and the Nitta–Chao predictions of density against pressure for different compositions in all binary systems at 298.15 K. Here it can be also observed the

TABLE 8
Modified Tait equation coefficients and deviations for density correlation of {dialkyl carbonate (1) + n-alkane (2)} mixtures.

x_1	$\rho_{00}/(g \cdot cm^{-3})$	$\rho_{01}/(g \cdot cm^{-3} \cdot K^{-1})$	C	B_0/MPa	$B_1/MPa \cdot K^{-1}$	$B_2/MPa \cdot K^{-2}$	$AAD^a/(g \cdot cm^{-3})$	$APD^a/\%$
				{Dimethyl carbonate + n-octane}				
0.0000	0.9392	$-8.0696 \cdot 10^{-4}$	$7.66 \cdot 10^{-2}$	785.20	-4.4452	$6.70 \cdot 10^{-3}$	$5.6 \cdot 10^{-4}$	$7.9 \cdot 10^{-2}$
0.0535	0.9641	$-8.6017 \cdot 10^{-4}$	$8.79 \cdot 10^{-2}$	394.07	-1.4666	$1.30 \cdot 10^{-3}$	$4.6 \cdot 10^{-4}$	$6.3 \cdot 10^{-2}$
0.0978	0.9679	$-8.4713 \cdot 10^{-4}$	$7.69 \cdot 10^{-2}$	382.47	-1.6864	$2.00 \cdot 10^{-3}$	$2.4 \cdot 10^{-4}$	$3.3 \cdot 10^{-2}$
0.3935	1.0611	$-9.3490 \cdot 10^{-4}$	$7.48 \cdot 10^{-2}$	2.0379	0.7340	$-1.80 \cdot 10^{-3}$	$8.6 \cdot 10^{-4}$	$1.1 \cdot 10^{-1}$
0.4960	1.1189	$-1.0274 \cdot 10^{-3}$	$7.90 \cdot 10^{-2}$	234.80	-0.6148	$1.00 \cdot 10^{-4}$	$6.6 \cdot 10^{-4}$	$7.9 \cdot 10^{-2}$
0.5475	1.1556	$-1.0926 \cdot 10^{-3}$	$8.68 \cdot 10^{-2}$	679.81	-3.3167	$4.30 \cdot 10^{-3}$	$1.7 \cdot 10^{-4}$	$2.0 \cdot 10^{-2}$
0.5937	1.1624	$-1.0600 \cdot 10^{-3}$	$7.66 \cdot 10^{-2}$	259.43	-0.8516	$6.00 \cdot 10^{-4}$	$9.6 \cdot 10^{-4}$	$1.1 \cdot 10^{-1}$
0.7002	1.2204	$-1.1132 \cdot 10^{-3}$	$7.79 \cdot 10^{-2}$	298.19	-1.0429	$9.00 \cdot 10^{-4}$	$1.2 \cdot 10^{-4}$	$1.3 \cdot 10^{-2}$
0.8013	1.2520	$-1.0700 \cdot 10^{-3}$	$3.71 \cdot 10^{-2}$	40.116	-0.0601	$7.57 \cdot 10^{-6}$	$1.0 \cdot 10^{-3}$	$1.1 \cdot 10^{-1}$
0.8979	1.3703	$-1.2678 \cdot 10^{-3}$	$8.96 \cdot 10^{-2}$	588.05	-2.5327	$2.90 \cdot 10^{-3}$	$1.3 \cdot 10^{-4}$	$1.3 \cdot 10^{-2}$
0.9502	1.3782	$-1.1836 \cdot 10^{-3}$	$6.20 \cdot 10^{-2}$	-74.881	1.0735	$-2.10 \cdot 10^{-3}$	$4.7 \cdot 10^{-4}$	$4.5 \cdot 10^{-2}$
1.0000	1.4629	$-1.3414 \cdot 10^{-3}$	$8.75 \cdot 10^{-2}$	612.57	-2.6318	$3.00 \cdot 10^{-3}$	$4.4 \cdot 10^{-4}$	$4.0 \cdot 10^{-2}$
				(Dimethyl carbonate + n-decane)				
0.0000	0.9545	$-7.6632 \cdot 10^{-4}$	$7.88 \cdot 10^{-2}$	228.25	-0.5583	$1.00 \cdot 10^{-4}$	$1.4 \cdot 10^{-4}$	$1.9 \cdot 10^{-2}$
0.0438	0.9609	$-7.6989 \cdot 10^{-4}$	$7.70 \cdot 10^{-2}$	667.01	-3.4957	$5.00 \cdot 10^{-3}$	$1.1 \cdot 10^{-4}$	$1.5 \cdot 10^{-2}$
0.1100	0.9667	$-7.5488 \cdot 10^{-4}$	$6.78 \cdot 10^{-2}$	-122.35	1.5094	$-3.00 \cdot 10^{-3}$	$6.6 \cdot 10^{-4}$	$8.7 \cdot 10^{-2}$
0.2348	1.0097	$-8.3479 \cdot 10^{-4}$	$7.70 \cdot 10^{-2}$	558.56	-2.8052	$3.90 \cdot 10^{-3}$	$2.5 \cdot 10^{-4}$	$3.2 \cdot 10^{-2}$
0.3516	1.0466	$-8.8364 \cdot 10^{-4}$	$7.82 \cdot 10^{-2}$	362.14	-1.4539	$1.60 \cdot 10^{-3}$	$3.7 \cdot 10^{-4}$	$4.7 \cdot 10^{-2}$
0.3944	1.0636	$-9.0778 \cdot 10^{-4}$	$7.61 \cdot 10^{-2}$	2646.3	-16.6783	$2.69 \cdot 10^{-2}$	$1.3 \cdot 10^{-4}$	$1.6 \cdot 10^{-2}$
0.5570	1.1938	$-1.2135 \cdot 10^{-3}$	$8.30 \cdot 10^{-2}$	-1092.0	9.0833	$-1.73 \cdot 10^{-2}$	$8.9 \cdot 10^{-4}$	$1.0 \cdot 10^{-1}$
0.8035	1.2856	$-1.1848 \cdot 10^{-3}$	$7.67 \cdot 10^{-2}$	-2186.4	15.5975	$-2.70 \cdot 10^{-2}$	$9.5 \cdot 10^{-4}$	$9.9 \cdot 10^{-2}$
0.9500	1.3993	$-1.2672 \cdot 10^{-3}$	$8.38 \cdot 10^{-2}$	386.39	-1.2985	$1.00 \cdot 10^{-3}$	$6.2 \cdot 10^{-5}$	$6.0 \cdot 10^{-3}$
				(Diethyl carbonate + n-octane)				
0.0522	0.9526	$-8.2110 \cdot 10^{-4}$	$8.01 \cdot 10^{-2}$	473.90	-2.2968	$3.10 \cdot 10^{-3}$	$5.9 \cdot 10^{-4}$	$8.2 \cdot 10^{-2}$
0.1042	0.9683	$-8.4030 \cdot 10^{-4}$	$7.97 \cdot 10^{-2}$	252.11	-0.8118	$6.00 \cdot 10^{-4}$	$3.8 \cdot 10^{-4}$	$5.1 \cdot 10^{-2}$
0.1671	0.9885	$-8.6734 \cdot 10^{-4}$	$8.19 \cdot 10^{-2}$	227.98	-0.5859	$1.00 \cdot 10^{-4}$	$4.4 \cdot 10^{-4}$	$5.8 \cdot 10^{-2}$
0.3220	1.0206	$-8.5995 \cdot 10^{-4}$	$6.94 \cdot 10^{-2}$	77.770	0.0921	$-6.00 \cdot 10^{-4}$	$2.7 \cdot 10^{-4}$	$3.4 \cdot 10^{-2}$
0.3657	1.0523	$-9.3082 \cdot 10^{-4}$	$7.78 \cdot 10^{-2}$	325.69	-1.2723	$1.30 \cdot 10^{-3}$	$6.9 \cdot 10^{-5}$	$8.7 \cdot 10^{-3}$
0.5075	1.1023	$-9.7789 \cdot 10^{-4}$	$7.91 \cdot 10^{-2}$	433.65	-1.9286	$2.30 \cdot 10^{-3}$	$4.6 \cdot 10^{-4}$	$5.6 \cdot 10^{-2}$
0.6922	1.1602	$-9.9208 \cdot 10^{-4}$	$8.77 \cdot 10^{-2}$	-1005.1	7.5595	$-1.32 \cdot 10^{-2}$	$4.9 \cdot 10^{-4}$	$5.5 \cdot 10^{-2}$
0.8002	1.2178	$-1.0734 \cdot 10^{-3}$	$8.18 \cdot 10^{-2}$	338.67	-1.1425	$9.00 \cdot 10^{-4}$	$4.1 \cdot 10^{-4}$	$4.5 \cdot 10^{-2}$
0.9206	1.2813	$-1.1469 \cdot 10^{-3}$	$8.99 \cdot 10^{-2}$	665.60	-3.0107	$3.60 \cdot 10^{-3}$	$4.7 \cdot 10^{-4}$	$4.9 \cdot 10^{-2}$
0.9459	1.2797	$-1.1095 \cdot 10^{-3}$	$8.43 \cdot 10^{-2}$	11.631	1.1432	$-3.00 \cdot 10^{-3}$	$1.6 \cdot 10^{-4}$	$1.7 \cdot 10^{-2}$
1.0000	1.3055	$-1.1288 \cdot 10^{-3}$	$8.55 \cdot 10^{-2}$	464.20	-1.8622	$2.00 \cdot 10^{-3}$	$2.7 \cdot 10^{-4}$	$2.7 \cdot 10^{-2}$
				(Diethyl carbonate + n-decane)				
0.0538	0.9621	$-7.6783 \cdot 10^{-4}$	$7.81 \cdot 10^{-2}$	242.78	-0.6592	$3.00 \cdot 10^{-4}$	$4.3 \cdot 10^{-4}$	$5.7 \cdot 10^{-2}$
0.1716	0.9930	$-8.1075 \cdot 10^{-4}$	$7.32 \cdot 10^{-2}$	-539.57	4.4544	$-8.10 \cdot 10^{-3}$	$6.7 \cdot 10^{-4}$	$8.7 \cdot 10^{-2}$
0.2151	1.0024	$-8.1953 \cdot 10^{-4}$	$7.67 \cdot 10^{-2}$	301.91	-1.0660	$9.00 \cdot 10^{-4}$	$7.1 \cdot 10^{-4}$	$9.2 \cdot 10^{-2}$
0.3257	1.0330	$-8.5557 \cdot 10^{-4}$	$7.57 \cdot 10^{-2}$	278.66	-0.9290	$7.00 \cdot 10^{-4}$	$5.5 \cdot 10^{-4}$	$6.8 \cdot 10^{-2}$
0.5032	1.0653	$-8.4584 \cdot 10^{-4}$	$6.75 \cdot 10^{-2}$	123.20	-0.2170	$-1.54 \cdot 10^{-5}$	$2.6 \cdot 10^{-4}$	$3.1 \cdot 10^{-2}$
0.5482	1.0956	$-9.1429 \cdot 10^{-4}$	$7.51 \cdot 10^{-2}$	513.96	-2.5579	$3.50 \cdot 10^{-3}$	$7.8 \cdot 10^{-4}$	$9.3 \cdot 10^{-2}$
0.7985	1.2015	$-1.0353 \cdot 10^{-3}$	$8.13 \cdot 10^{-2}$	360.25	-1.2793	$1.10 \cdot 10^{-3}$	$1.5 \cdot 10^{-4}$	$1.6 \cdot 10^{-2}$
0.8989	1.2234	$-9.9118 \cdot 10^{-4}$	$6.30 \cdot 10^{-2}$	98.751	-0.1083	$-1.00 \cdot 10^{-4}$	$4.3 \cdot 10^{-4}$	$4.6 \cdot 10^{-2}$
0.9487	1.2497	$-1.0151 \cdot 10^{-3}$	$6.25 \cdot 10^{-2}$	15.067	0.4683	$-1.10 \cdot 10^{-3}$	$4.1 \cdot 10^{-4}$	$4.3 \cdot 10^{-2}$

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

highest density values for the (dimethyl carbonate + n-decane) binary mixtures. Nitta–Chao model predict correctly the high pressure density for all systems studied especially the (diethyl carbonate + n-alkanes) binary mixtures, although for the pure dimethyl carbonate and mixtures rich compositions in this compound the deviations are higher.

Figure 3 shows Tait correlations and Nitta-Chao predictions for an approximately equimolar mixture in each binary mixture at (288.15, 298.15, and 308.15) K. The mean APD for all binary systems studied in overall range compositions were 0.051% and 0.68% using Tait equation correlation and Nitta–Chao prediction, respectively. The maximum APD was obtained for (dimethyl carbonate + n-octane) binary system in both method used. These values are 0.107% and 1.10% for Tait equation correlation and Nitta–Chao prediction, respectively. From this figure it can be observed a good agreement between correlation and the predictions for all

systems studied, however the Tait correlation shows the best results.

Figure 4 shows the isothermal compressibility κ_T changes with pressure calculated by equation (4) and predicted by Nitta–Chao model at (288.15, 298.15, and 308.15) K, and at a fixed molar compositions in the (diethyl carbonate + n-decane) binary mixture. The κ_T decreased with an increase in pressure and with a decrease in temperature due to the less intermolecular space and the less possibility of approximation. The same results have been obtained for the remaining (dialkyl carbonate + n-alkane) binary mixtures studied in this work. The isothermal compressibility at the different temperatures converges at the high pressure due a compact molecular packaging and increased with the higher carbonate compositions.

Increasing the alkyl chain length the isothermal compressibility values of the alkyl carbonate and their mixtures with n-octane and
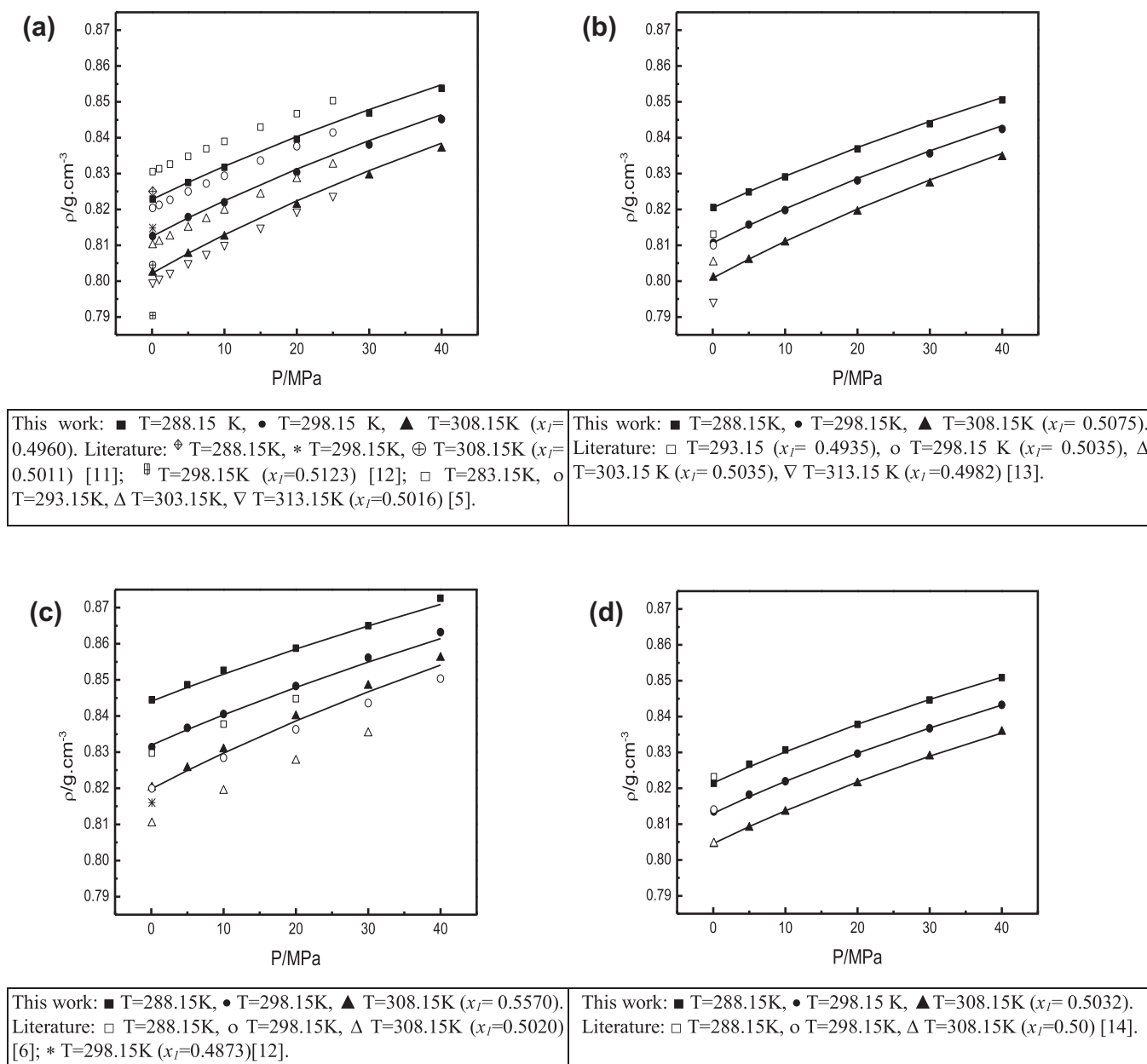

This work: ■ T=288.15 K, ● T=298.15 K, ▲ T=308.15K (x_1= 0.4960). Literature: ⬦ T=288.15K, ∗ T=298.15K, ⊕ T=308.15K (x_1= 0.5011) [11]; ⊞ T=298.15K (x_1=0.5123) [12]; □ T=283.15K, ○ T=293.15K, △ T=303.15K, ▽ T=313.15K (x_1=0.5016) [5].

This work: ■ T=288.15K, ● T=298.15K, ▲ T=308.15K (x_1= 0.5075). Literature: □ T=293.15 (x_1= 0.4935), ○ T=298.15 K (x_1= 0.5035), △ T=303.15 K (x_1= 0.5035), ▽ T=313.15 K (x_1=0.4982) [13].

This work: ■ T=288.15K, ● T=298.15K, ▲ T=308.15K (x_1= 0.5570). Literature: □ T=288.15K, ○ T=298.15K, △ T=308.15K (x_1=0.5020) [6]; ∗ T=298.15K (x_1=0.4873)[12].

This work: ■ T=288.15K, ● T=298.15 K, ▲T=308.15K (x_1= 0.5032). Literature: □ T=288.15K, ○ T=298.15K, △ T=308.15K (x_1=0.50) [14].

FIGURE 1. Comparison between experimental high pressure binary mixtures density ρ (filled symbols) at fixed dialkyl carbonate compositions x_1 against pressure P of: (a) (dimethyl carbonate + n-octane); (b) (diethyl carbonate + n-octane); (c) (dimethyl carbonate + n-decane); (d) (diethyl carbonate + n-decane). Experimental data: symbols. Tait correlations: lines.
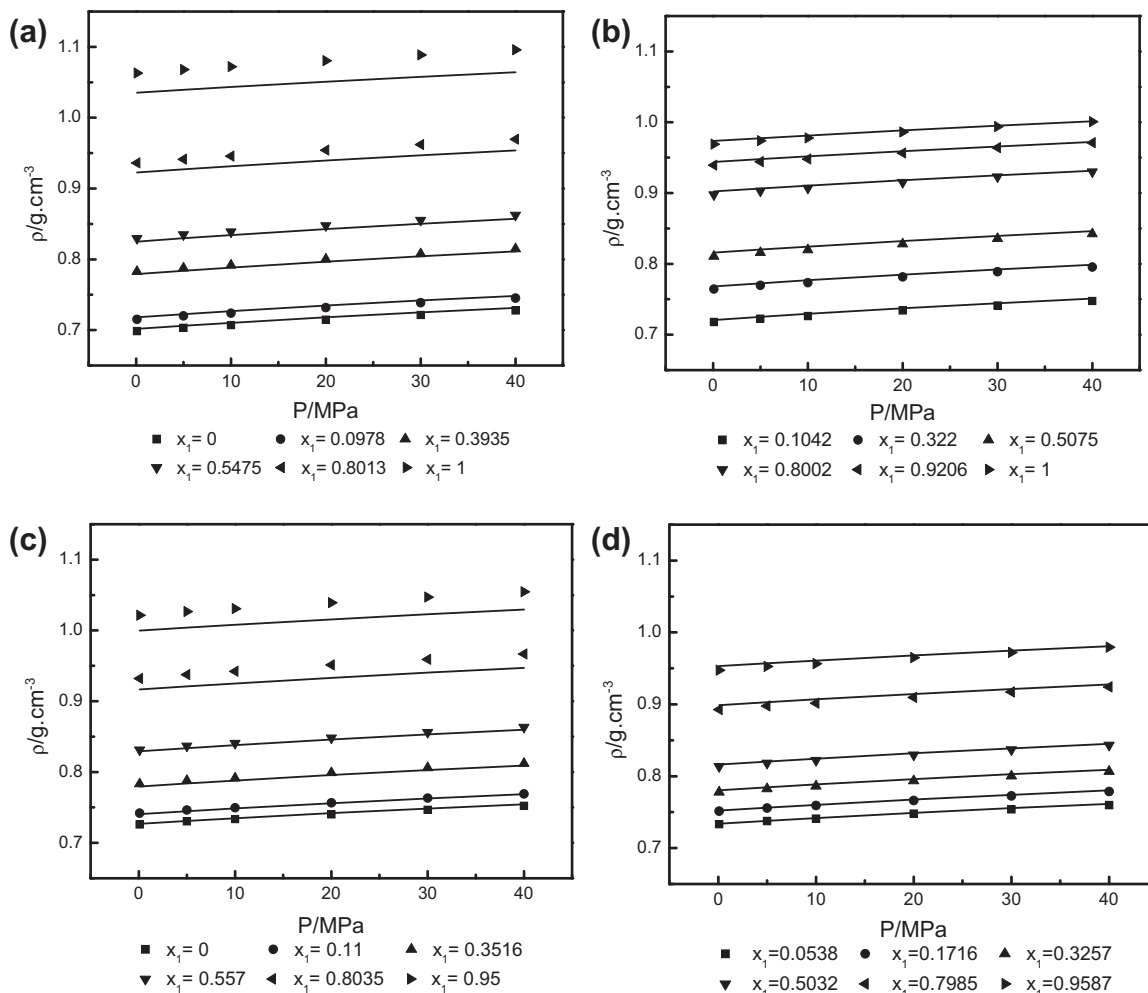
FIGURE 2. High pressure density ρ of {dialkyl carbonate (1) + n-alkane (2)} binary mixtures against pressure P for: (a) (dimethyl carbonate + n-octane), (b) (diethyl carbonate + n-octane), (c) (dimethyl carbonate + n-decane), (d) (diethyl carbonate + n-decane) at T = 298.15 K. Experimental data: symbols. Nitta–Chao predictions: lines.

n-decane increase. Also, the k_T values increase with the decrease of dialkyl carbonate concentration. Regarding pure components, the isothermal compressibility values increases with a decrease of density values. These results are in agreement with Comuñas et al. [7] who have studied the behavior of pure dialkyl carbonate.

Figure 5 shows the isobaric thermal expansion α_p against pressure calculated by equation (5) and predicted by Nitta–Chao model, at the different temperatures studied and a fixed molar fraction for (diethyl carbonate + n-decane) binary mixtures. The α_p has the same behavior that k_T with regard to temperature and pressure for all systems studied in this work. However, in some compositions, it can be found an intersection point of isotherms, which is related to the minimum of isobaric heat capacity as reported Comuñas et al. [7]. The isobaric thermal expansion is independent of temperature in the crossing point pressure and increase with the concentration of dialkyl carbonate for all systems.

Figure 6 shows the trend of internal pressure π with pressure calculated by equation (6) and the Nitta–Chao predictions for (diethyl carbonate + n-decane) for a fixed molar fraction at different temperatures. This figure provides qualitative information about the microscopic properties of the liquid [17]. This property depends of pressure and temperature and its behavior can be explained in terms of competition between the attractive and the repulsive internal energy terms. At low density, the internal en-

ergy can be represented correctly by an attractive term; while at high density the repulsive energy are more significant, obtaining an increment of the internal energy. From this figure it can be seen an increase of the internal pressure with an increment of pressure in all temperatures studied, typical for the non associated liquids [24] and a decrease of this property with an increase of temperature. This behavior is present again in all systems studied. Figures 4 and 5 show a good agreement for the Nitta–Chao predictions with the experimental data in the isobaric thermal expansion and isothermal compressibility, respectively. However, from Figure 6 it can seen a less accurate in the predictions for the internal pressure, but it can reproduce correctly the behavior with an APD low. For example, the mean APD between the experimental and predicted Nitta–Chao model applied to derived properties for (diethyl carbonate + n-decane) binary systems showed in figures 4, 5, 6 are: 3.49% for isothermal compressibility, 1.73% for isobaric thermal expansion, and 3.79% for internal pressure, respectively.

As isobaric thermal expansion, the internal pressure of (dimethyl carbonate + n-alkane) binary mixtures is higher than (diethyl carbonate + n-alkane) binary mixtures due the insertion of methylene groups that reduces the internal pressure. This result is in agreement with those reported by Comuñas et al. [7] for pure compounds between (283.15 and 353.15) K and pressures up to 60 MPa.
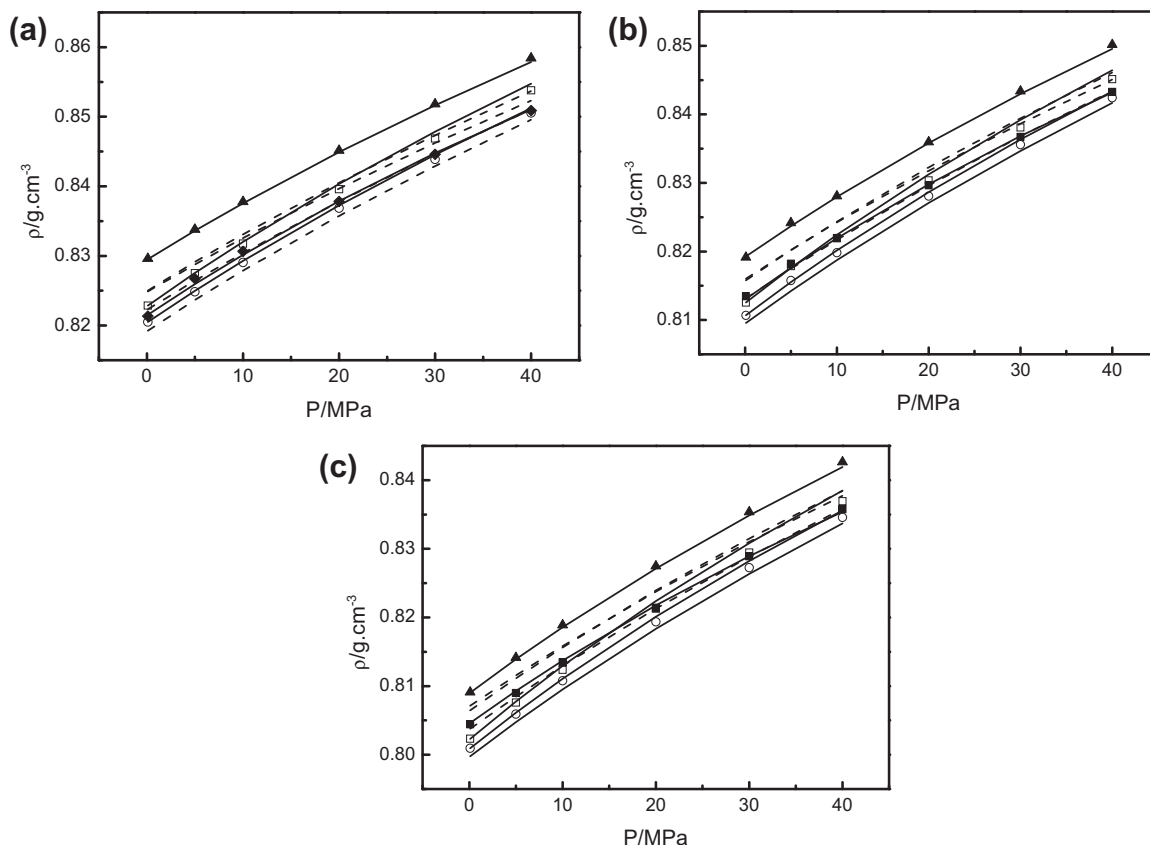
FIGURE 3. Comparison among experimental data (symbols), Nitta–Chao prediction (dashed lines) and Tait correlation (solid lines) density ρ against pressure P at different temperatures: (a) T = 288.15 K, (b) T = 298.15 K and (c) T = 308.15 K for {dimethyl carbonate (1) + n-octane (2)} ($\square$, x_1 = 0.4960); {diethyl carbonate (1) + n-octane (2)} (o, x_1 = 0.5075); {dimethyl carbonate (1) + n-decane (2)} ($\blacktriangle$, interpolated values at x_1 = 0.50); {diethyl carbonate (1) + n-decane (2)} ($\blacksquare$, x_1 = 0.5032) binary mixtures.
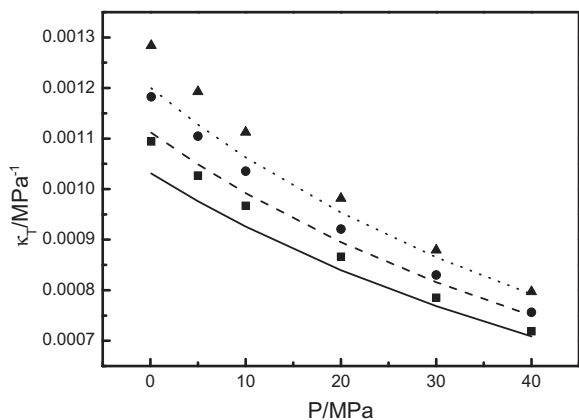
FIGURE 4. Comparison between experimental data (symbols) and Nitta–Chao prediction (lines) for isothermal compressibility κ_T against pressure P of {diethyl carbonate (1) + n-decane (2)} system at x_1 = 0.3257. From lower to higher κ_T the temperatures correspond to (288.15, 298.15, and 308.15) K.
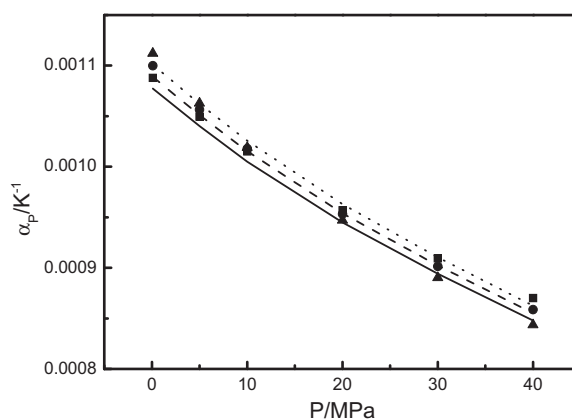
FIGURE 5. Comparison between experimental data (symbols) and Nitta–Chao prediction (lines) for isobaric thermal expansion coefficient α_P against pressure P of {diethyl carbonate (1) + n-decane (2)} system at x_1 = 0.3257. From lower to higher α_P the temperatures are (288.15, 298.15, and 308.15) K.

6. Conclusion

New experimental high-pressure density data are reported for dimethyl carbonate, diethyl carbonate, n-octane, n-decane and their binary mixtures: (dimethyl carbonate + n-octane), (diethyl carbonate + n-octane), (dimethyl carbonate + n-decane), and (diethyl carbonate + n-decane) at (288.15, 298.15, and 308.15) K and pressures between (0.1 and 40) MPa. Isobaric thermal expansivity coefficient, isothermal compressibility coefficient and inter-

nal pressure were also studied in all composition, temperature and pressure range. These data are valuable to obtain an adequate description of thermophysical behavior of mixtures containing (dialkyl carbonate + n-alkanes) useful in the fuel field. All experimental data were well correlated using Tait equation. Regarding predictions about the systems, the Nitta–Chao group contribution model describes correctly the high pressure density and their derivate properties such as isobaric thermal expansivity coefficient, isothermal compressibility coefficient and internal pressure of
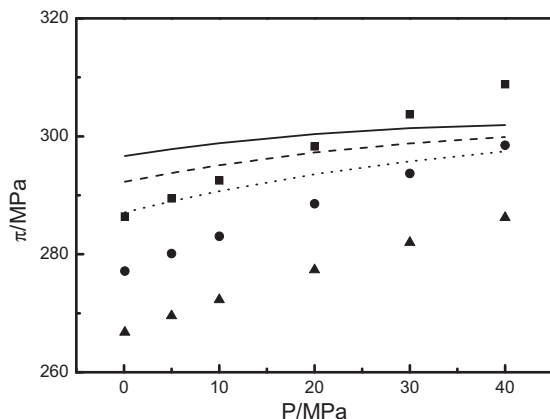
FIGURE 6. Comparison between experimental data (symbols) and Nitta–Chao prediction (lines) for internal pressure π against pressure P of {diethyl carbonate (1) + n-decane (2)} system at $x_1 = 0.3257$. From lower to higher π the temperatures correspond to (288.15, 298.15, and 308.15) K.

the pure components and the (dialkyl carbonate + n-alkane) binary mixtures. The Nitta-Chao model can be useful to predict different mixtures at those studied containing methyl, methylene, and carbonate groups.

Acknowledgments

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