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Modelling and Experimental Thermodynamic Data of Hydroxylic Compounds (C_1-C_6) as a Function of Temperature

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Abstract

Alcohols have a long history of several uses worldwide. Because of their relatively low toxicity compared with other many chemical compounds and ability to dissolve non-polar substances, alcohols can be found into beverages for adults, used as combustion engine fuel, as excipient in medical drugs, as component into personal-care products and in many scientific and industrial applications. One of the key problems of the chemical industry is the lack of available physical properties data for equipment industrial design and improvement of theoretical models for simulation. The present work deals with the modelling and experimental measurement (density and ultrasonic velocity) of thermophysical properties of short chain hydroxylic compounds (C_1-C_6), making a contribution with quality data to the available thermodynamic databases. Fitting equations were applied to the experimental data in order to correlate for later computer based design. Different derived magnitudes were computed from the experimentally measured density and ultrasonic velocity, due to their importance for theoretical calculations and development of new models. The estimation of the studied properties was made by the application of different theoretical procedures. A wide comparison was made with available open literature, being evident the lack of reliable information in the ranges studied until now.

Keywords: *Alcohol; thermodynamic properties; temperature; theoretical model; prediction*

1. Introduction

Modern development in chemical industry requires the minimization of environmental impact using clean processes and new production strategies. An important part of the environmental impact is related to the nature of the solvents used, as well as, their potential hazards profile [1-3]. In recent years it has boosted the use of water and alcohols in industrial processes due to its high polar character, low cost, environmental low impact, wide availability and high capacity solvent [4-5]. Alcohols can be used as a beverage, as combustion engine fuel and for different scientific, medical, and industrial applications. Methanol is made primarily from natural gas, and is an intermediate material to produce thousands of derivative products evolving key chemicals (acetic acid, formaldehyde, ethanoic acid and different methyl esters), acrylic plastics, synthetic fibers, adhesives, ink, paints, construction materials, agrichemicals and pharmaceutical compounds. The versatility of this alcohol is making it a promising fuel resource as core energy carrier for factories and electricity generation, as well as, for portable power sources (direct methanol fuel cells) [6]. Ethanol in the form of alcoholic beverages has been consumed by humans since pre-historic times. It is possible to trace alcoholic beverages made by humans to about nine millennia ago but probably, alcoholic products based on fruit juice fermentation may be consumed many centuries earlier [7], and today it is widely associated with socialising for adult population into occidental countries. Different studies in the last few years have shown some potential health benefits under moderate consumption conditions [8]. Ethanol can be used as promising alternative to fossil fuel or fuel additive for internal combustion motors, due to it can be obtained from renewable biomass sources. Fuel performance can be increased in forced induction internal combustion engines by injecting alcohols into the air intake after the turbocharger has pressurized the air. Brazil is the world´s second largest producer of ethanol fuel (30094 millions of litres in 2018-2019), rising 23.3% in the last period, representing 27.7% of the total produced ethanol fuel. Brazil´s fuel program is based on the most efficient agricultural technology for sugarcane cultivation; however any authors consider that this model is only sustainable under advanced agro industrial processes, cheap feedstock and giant amount of available land. Since 1979, Brazil is the only country in the world that uses hydrated ethanol as fuel for combustion engines adapted specifically for mixed use (gasoline, ethanol or any degree of mixture (commonly called gasohol)), currently 85% of the vehicles in circulation in the country use this kind of adapted engine. Today, there are already different successfully experiences of application of hydrated ethanol for motorcycles in Brasil (since 2009, biofuel engine of Honda and Yamaha) or as an additive for diesel engines or as a single fuel (since 1997, MAD7 (diesel-blended alcohol), since 2006, Bioethanol for

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Sustainable Transport, BEST-Program, E95 for buses (95% ethanol and 5% additives)) or for air transport (since 2005, different EMBRAER projects, Ipanema EMB202A or E195, for example). Besides ethanol, different studies are available evolving different mixtures of alcohols as promising alternative fuel [9-20]. Propanol is used as solvent (as entrainer for azeotropic distillation, for printing inks, electrodeposition paints), personal care products (soaps, antifreezer, lacquer formulation, etc) and cleaning products (window cleaners, adhesives, etc) and as intermediate product for halides, propyl amine, propyl acetate, esters and ethers production. Also is used for medical applications (as antiseptic, hand-sanitizer, nebulizer, pain relief medication and supraventricular arrhythmias/ventricular tachycardias treatment) and as constituent of many kinds cosmetics. Alcohol beverages nearly always gather propanol as fermentation component, as well as in many foodstuff and non-alcoholic drinks, being an important element of the flavor profile. Despite uses and applications of propanol are rising significantly, the cost of production is too expensive for a massive consumption as a combustion fuel but promising alternatives are being proposed for direct fuel cells [21-23]. Butanol is an important commodity in manufacturing industry (used in polymers, lubricants, brake fluids, synthetic rubber, as polishing and cleaning products, and as artificial food flavoring), cosmetic laboratories (used for soaps, shampoo, and personal-care products) and chemical industry (as intermediate to produce other compounds, as amino resins, different acetates and amines, glycol ether and acrylate esters). As potential fuel for combustion engines, butanol is an alternative fuel that offers high energy content, fewer emissions and lower corrosion [24]. Fermentative production of butanol for application as feedstock or biofuel is regarded as a promising renewable technology, but for the moment remains a barrier for a cost-effective production [25-26].

Higher alcohols such as pentanol chemicals are part of the next generation of biofuels, due to they provide better energy content and fuel properties (lower vapor pressure, higher octane number, higher heat of combustion, lower corrosion, lower potential for groundwater contamination and higher motor efficiency) than lower alcohols. Biodiesel–higher alcohol blends can be used in diesel engines without any engine modification. Short alcohols are soluble in water, but mainly those of longer structure show relatively insoluble trend into polar environment, avoiding problems of engine power due to water content into alcohols and potential groundwater pollution, moreover, these heavier alcohols show lower levels of corrosion and higher heat of combustion as the size of aliphatic chains increases. Research of pure combustion of higher alcohols for internal combustion engines is actually in progress. Pentanol and other higher alcohols can are obtained by fermentation in a restricted quantity being considered as secondary products. Currently, the principal method of production is related to the reaction of CO and H_2 and an alcohol, occurring the reaction under Cu/ZnO catalyzed conditions [27-31]. Other higher alcohol as phenylmethanol is commonly applied as solvent into inks, paints and epoxy resins industries. It is also used as flavour compound for electronic cigarettes and offers different potential uses as anesthetic, antimicrobial, repellent and dye solvent [32-33]. From a general point of view, alcohols have wide applications in industry and science as reagents (deprotonation, nucleophilic substitution, dehydration, esterification or oxidation processes) or solvents [34]. Due to its low toxicity and ability to dissolve non-polar substances, can be used as a solvent in medical drugs, first aid products, cleaning agent and perfumes. Mainly, ethanol can be used as an antiseptic and alcohol-based soaps and alcohol gels have become common as hand sanitizers, cleaning products and are convenient because they do not require drying due to the low vapour pressure of these compounds [35-38].

Besides its own practical importance, density and ultrasonic velocity are two key magnitudes closely linked with the determination of Henry's law constants and air-water partition coefficients, mass transfer coefficient measurement and calorimetric studies by means of Maxwell's coefficients. A considerable amount of data is available for organic hydrocarbons in open databases, which are of major environmental and health concern. Less attention has been paid to hydroxylic compounds, for which only a few number of wide experimental collections of data are available in the literature, as well as, accurate studies related to the dependence of their properties with temperature, pressure or composition. Moreover, it can be observed a considerable lack of accuracy or thermodynamic consistency in some open data literature, which is due to experimental errors, impurities of chemicals or differences on technical devices used for measuring. A worse perspective is obtained for mixture references owed to the recent development of accurate techniques, the relatively important non-ideality of such compounds into mixture, as well as, the time-consuming nature of the experimental measuring procedures.

Different previous published works report data compilations of physical and thermal properties of hydroxylic compounds but this information is not systematic, it can be found disperse and many properties have not been studied in a wide extension, mainly those of acoustic nature. This kind of information is of high interest for the understanding of the evolution of flexibility, package trend, hydrophobicity and polar-hydrogen bond potential as a function of molecular structure, as well as, for the development of group contribution methods for prediction of thermophysical properties. All chemicals selected for this study contain an unique hydroxylic group and aliphatic or aromatic residual structures of low molar mass.

In response to this concern, our research group has started determining multicomponent thermodynamics (phase equilibria, reology, acoustical, optical, volumetric and calorimetric magnitudes [39-50] in order to optimize simulation studies and understand the mixing mechanisms into complex mixtures.

With these facts in mind, as a continuation of our scientific work investigating physical properties related to characterization of compounds of industrial interest, we present the temperature dependence of density and ultrasonic velocity at the range of temperature 278.15-323.15 K and atmospheric pressure of a wide collection of alcohols (methanol, ethanol, propan-1-ol, propan-2-ol, butan-1-ol, butan-2-ol, 2-methyl-propan-1-ol, 2-methyl-propan-2-ol, pentan-1-ol, 2-methyl-butan-1-ol, 3-

methyl-butan-1-ol, and phenylmethanol). From the experimental data, temperature dependent polynomials were fitted, the corresponding parameters being gathered. Different derived properties were computed from density and ultrasonic velocity data, due to their importance in the study of the thermodynamic trend and theoretical calculations. Because of the expense of the experimental measurement of such data and current processes design is strongly computer oriented, consideration was also given to how accurate different theoretical methods work by comparison with the measured experimental data. For density estimation, a simplification of the Nasrifar–Moshfeghian liquid density correlation (MNM method) was applied, replacing the Mathias and Copeman temperature-dependent term with the original Soave–Redlich–Kwong equation of state (SRK EOS) temperature-dependent term [51]. This replacement has overcome the limitations in use for the original model, which were due to the Mathias and Copeman vapor pressure dependent parameters. The Rackett equation of state and its modification was also tested [52-53], as well as other different methods (Bradford-Thodos, Riedel, Narsimhan, Yen-Woods, Bhirud and Campbell-Thodos models) [54-59], in order to analyze how accurate densities are predicted.

The Collision Factor Theory (CFT) was applied to estimate the isentropic compressibility of these compounds [60] using the estimated collision factor for pure compounds. Satisfactory predictions were obtained for both properties, a good accuracy being obtained for a wide range of temperatures. Finally, a wide comparison was made with disposable open literature for the studied compounds, an analysis being made of the obtained results.

2. Experimental

All chemical solvents used in the experimental studies were of Merck quality with richness better than 99.0 mol%. The pure components were stored in sun light protected form and constant humidity and temperature. Usual manipulation and purification in our experimental works was applied, as earlier explained [49-50]. The molar mass, open literature data and experimental results at standard condition are shown in Table 1. The densities and ultrasonic velocities of pure components were measured with an Anton Paar DSA-5000M vibrational tube densimeter and sound analyser, with a resolution of 10^{-5} gcm^{-3} and 1 ms^{-1}. The densimetry cell determines the densities of liquid mixtures by measuring electronically the period of a glass oscillator. The corresponding alcohol sample is introduced into a cell which can oscillate and whose frequency is influenced by the mass of the sample. The cell is a U-shaped tube which is brought to undamped oscillation by electronic means. Both straight sections of the U-shaped tube form the spring element of the oscillator. The direction of the oscillation lies in the same plane as the tube; if the oscillator has been filled with the sample at least up to the mounting points, then the same known volume of sample also oscillates. The density of the alcohol can be calculated from the oscillation period by considering it as a function of device constants, sample volume and temperature. The ultrasonic cell determines the ultrasonic velocity of mixtures by means of the sing-around technique. Low intensity ultrasound is used in a very wide range of applications in industry. Many of the applications, such as the measure of density and porosity, involve the measurement of ultrasonic velocities or its attenuation. The review article by Lynnworth (1975) [81] discusses many of these applications. The principle of operation of the sing-around method in this system is that the received pulse triggers another pulse so that a repetitive trigger signal occurs at a rate equal to the reciprocal of the propagation time. The frequency and thus the period between trigger pulses can be very accurately measured and the system is easily automated. However, any timing delays associated with the electronics will show up as errors in the determination of transit time. These electrical delays may be minimized by appropriate signal processing. This system is easily good to 1% (this is dependent upon path length) for absolute measurements, but is several orders of magnitude more accurate when used as a comparison technique. Both experimental procedures are of wide application and have been applied successfully for different types of mixtures earlier [40, 49-50]. Apparatus calibration was performed periodically in accordance with vendor instructions using a double reference (Millipore quality water and ambient air at each temperature). Accuracy in the temperature of measurement was better than $\pm 10^{-2}$ K by means of a temperature control device that applies the Peltier principle to maintain isothermal conditions during the measurements.

For compact and smooth representation, the density and ultrasonic velocity of the chemicals were correlated as a function of temperature in accordance to the Eq. 1:

$$P = \sum_{i=0}^{N} A_i T^i \tag{1}$$

where the magnitude P is density (gcm^{-3}) or ultrasonic velocity (ms^{-1}), T is temperature in Kelvin and A_i are fitting parameters. N stands for the extension of the mathematical serie which was optimized by means of the Bevington test. Densities and ultrasonic velocity, as a function of temperature, are given in Table S1 as supplementary material. The fitting parameters were obtained by the unweighted least squared method applying a fitting Marquardt algorithm. The root mean square deviations were computed using Eq. 2, where z_{exp} and z_{pred} are the experimental and predicted values of the property, respectively, and n_{DAT} is the number of experimental data.

$$\sigma = \left(\frac{\sum_{i=1}^{n_{DAT}} \left(z_{exp} - z_{pred} \right)^2}{n_{DAT}} \right)^{1/2} \tag{2}$$

The fitting parameters and the corresponding deviations are gathered in Table 2. In Figures 1, 2 and 3, the temperature trend of density, ultrasonic velocity and isentropic compressibility (computed by the Newton-Laplace equation) are gathered. A decrease in the packing efficiency of chemicals by molecular kinetics results in a continuous diminution of density and ultrasonic velocity versus temperature, as observed into

Figures 1 and 2. The heavier hydroxylic compounds show the highest values of both magnitudes. Due to the inverse relation between these physical properties and isentropic compressibility (Newton-Laplace equation), this magnitude shows a rising tendency with temperature as gathered into Figure 3.

Table 1 Molar mass and experimental/open literature data for the studied compounds at 298.15 K.

component	M^a (kg/kmol)	ρ/(gcm^{-3}) exptl.	ρ/(gcm^{-3}) lit.	u/(ms^{-1}) exptl.	u/(ms^{-1}) lit.
Methanol	32.04	0.7866	0.7864[b]	1105.8	1102.3[b]
			0.7863[c]		1104.3[p]
			0.7866[d]		1104[q]
Ethanol	46.07	0.7884	0.7858[e]	1163.6	1143.1[e]
			0.7854[f]		1161.0[r]
			0.7852[g]		
Propan-1-ol	60.09	0.7994	0.8001[h]	1207.2	1205.4[h]
			0.7996[i]		1206.0[r]
			0.8008[t]		1207.2[t]
Propan-2-ol	60.09	0.7808	0.7813[j]	1139.8	1144.0[r]
			0.7809[k]		1137.3[t]
			0.7810[t]		
Butan-1-ol	74.12	0.8058	0.8057[i]	1201.6	1268.0[r]
			0.8057[j]		1240.1[s]
			0.8057[s]		1236.8[t]
			0.8059[t]		
Butan-2-ol	74.12	0.8027	0.8027[l]	1212.2	1211.6[n]
			0.8023[m]		1211.6[s]
			0.8024[s]		
2-Methyl-propan-1-ol	74.12	0.8042	0.7976[e]	1200.6	1185.6[e]
2-Methyl-propan-2-ol	74.12	0.8042	0.77548[n]	1184.9	1098.9[l]
Pentan-1-ol	88.15	0.8178	0.8109[e]	1280.3	1273.3[e]
			0.8111[t]		1273.3[t]
2-Methyl-butan-1-ol	88.15	0.8201	0.8147[e]	1246.6	1251.4[e]
			0,8152[s]		1254.5[s]
3-Methyl-butan-1-ol	88.15	0.8156	0.8063[e]	1243.9	1232.5[e]
Phenylmethanol	108.14	1.0472	1.0417[o]	1522.7	1532.4[o]

[61][a], [62][b], [63][c], [64][d], [65][e], [66][f], [67][g], [68][h], [69][i], [70][j], [71][k], [72][l], [73][m], [74][n], [75][o], [76][p], [77][q], [78][r], [79][s], [80][t]

3. Theoretical

3.1 Derived Properties

A frequently applied derived magnitude for chemicals is the temperature dependence of the volumetric trend which is expressed as isobaric expansibility (α). The open literature data normally give only these coefficients of pure compounds and its mixtures, showing the relative changes in density, calculated by means of $-(\Delta\rho/\rho)$ as a function of temperature and assuming that α remains constant in any range of temperature. This fact is due to the scarce availability of really accurate density data as a function of temperature. This magnitude may be computed as:

$$\alpha = -\left(\frac{\partial \ln\rho}{\partial T}\right)_P \qquad (3)$$

Considering the temperature dependence of density. Two tendencies are gather in terms of isobaric expansibility versus temperature. At first, those compounds of the lowest molar mass show a decreasing trend for rising temperatures, as methanol, ethanol, propan-1-ol, 2-methyl-propan-1-ol or 2-methyl-propan-2-ol. Those of higher molar mass show higher positive values and an opposite trend, increasing the isobaric expansibility when temperature rises, as observed into Figure 4.

The parameters derived from the experimental measured data were intermolecular free length (Lf), the van der Waals' constant (b), molecular radius (r), geometrical volume (B), molar surface area (Y), available volume (V_a), volume at absolute zero (V_0), molar sound velocity (Ra), collision factor (S) and specific acoustic impedance (Z), attending to the following set of equations:

$$L_f = \left(\frac{K}{u\cdot\rho^{1/2}}\right) \qquad (4)$$

$$b = \left(\frac{M}{\rho}\right) - \left(\frac{RT}{\rho\cdot u^2}\right)\cdot\left(\left[1+\frac{M\cdot u^2}{3RT}\right]^{1/2} - 1\right) \qquad (5)$$

$$r = \left(\frac{3b}{16\Pi N}\right)^{1/3} \qquad (6)$$

$$B = \left(\frac{4}{3}\right)\Pi r^3 N \qquad (7)$$

$$Y = \left(36\Pi N B^2\right)^{1/3} \qquad (8)$$

$$V_a = V\left(1-\left(\frac{u}{u_\infty}\right)\right) \qquad (9)$$

$$V_0 = V - V_a \qquad (10)$$

$$Ra = \frac{M\cdot u^{1/3}}{\rho} \qquad (11)$$

$$S = \frac{u\cdot V}{B\cdot u_\infty} \qquad (12)$$

$$Z = u\cdot\rho \qquad (13)$$

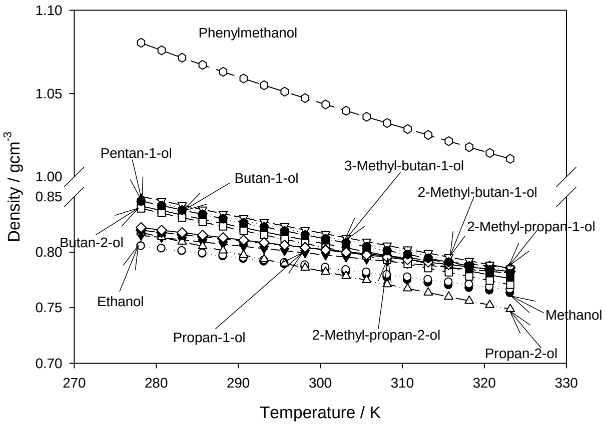

Figure 1. Experimental densities as a function of temperature: (●) methanol, (○) ethanol, (▼) propan-1-ol, (△) propan-2-ol, (■) butan-1-ol, (□) butan-2-ol (◆) 2-methyl-propan-1-ol, (◇) 2-methyl-propan-2-ol, (▲) pentan-1-ol, (▽) 2-methyl-butan-1-ol, (⬢) 3-methyl-butan-1-ol, (⬡) phenylmethanol.

	L_f (Å)	$b\cdot10^6$ (m$^3\cdot$mol^{-1})	$r\cdot10^3$ (nm)	$B\cdot10^6$ (m$^3\cdot$mol^{-1})	$Y\cdot10^{-8}$ (m^2)	$V_a\cdot10^6$ (m$^3\cdot$mol^{-1})	$V_0\cdot10^6$ (m$^3\cdot$mol^{-1})	$Ra\cdot10^3$ (m$^3\cdot$mol^{-1})$\cdot$(m$\cdot$s^{-1})$^{1/3}$
Methanol	0.210	35.281	3.168	8.820	8.3530	12.579	28.154	0.421
Ethanol	0.199	52.318	3.612	13.080	10.8621	15.936	42.497	0.615
Propan-1-ol	0.191	68.568	3.953	17.142	13.0085	18.455	56.718	0.800
Propan-2-ol	0.204	69.224	3.966	17.306	13.0914	21.987	54.469	0.799
Butan-1-ol	0.190	84.087	4.231	21.022	14.9049	22.754	68.638	0.972
Butan-2-ol	0.189	84.487	4.238	21.122	14.9512	22.238	69.509	0.978
2-Methyl-propan-1-ol	0.191	84.783	4.243	21.196	14.9861	23.008	69.158	0.980
2-Methyl-propan-2-ol	0.194	84.663	4.241	21.166	14.9719	23.910	68.254	0.975
Pentan-1-ol	0.178	100.423	4.489	25.106	16.7765	21.532	86.248	1.170
2-Methyl-butan-1-ol	0.182	99.917	4.482	24.979	16.7201	23.740	83.748	1.157
3-Methyl-butan-1-ol	0.183	100.442	4.490	25.110	16.7786	24.052	84.028	1.162
Phenylmethanol	0.132	98.252	4.457	24.563	16.5338	4.986	98.280	1.188

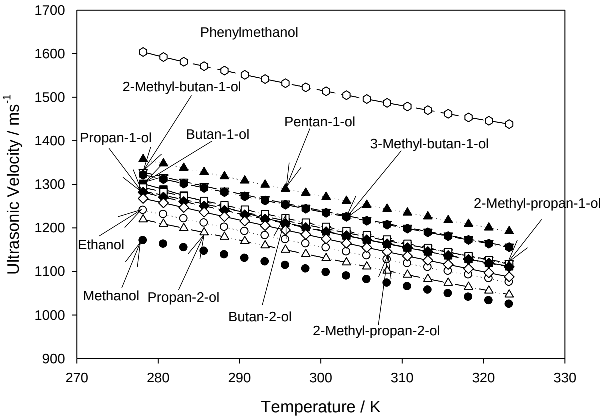

Figure 2. Experimental ultrasonic velocities as a function of temperature: (●) methanol, (○) ethanol, (▼) propan-1-ol, (△) propan-2-ol, (■) butan-1-ol, (□) butan-2-ol (◆) 2-methyl-propan-1-ol, (◇) 2-methyl-propan-2-ol, (▲) pentan-1-ol, (▽) 2-methyl-butan-1-ol, (⬢) 3-methyl-butan-1-ol, (⬡) phenylmethanol.

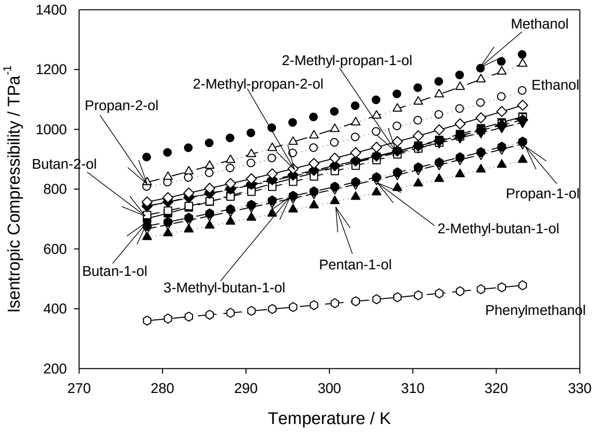

Figure 3. Experimental isentropic compressibilities as a function of temperature: (●) methanol, (○) ethanol, (▼) propan-1-ol, (△) propan-2-ol, (■) butan-1-ol, (□) butan-2-ol (◆) 2-methyl-propan-1-ol, (◇) 2-methyl-propan-2-ol, (▲) pentan-1-ol, (▽) 2-methyl-butan-1-ol, (⬢) 3-methyl-butan-1-ol, (⬡) phenylmethanol.

Table 2 Parameters of Eq. 1 at the range 278.15-323.15 K and root mean square deviations (Eq. 2).

	$\rho/(gcm^{-3})$				
	A_0	A_1	A_2	A_3	σ
Methanol	1.069428e+0	-9.494163e-4	4.638741e-9	-4.967753e-12	1.573041e-7
Ethanol	0.920656+0	1.743948e-4	-2.732918e-6	2.214711e-9	1.398198e-7
Propan-1-ol	0.806336+0	1.806446e-3	-9.767445e-6	1.217852e-8	9.711496e-6
Propan-2-ol	8.919535e-1	6.075419e-4	-5.089743e-6	6.045728e-9	1.003667e-5
Butan-1-ol	7.987042e-1	1.901449e-3	-1.005912e-5	1.261663e-8	1.147432e-5
Butan-2-ol	7.629473e-1	2.026794e-3	-9.571699e-6	1.080296e-8	1.079584e-5
2-Methyl-propan-1-ol	8.174602e-1	1.659479e-3	-9.010455e-6	1.105328e-8	1.712999e-5
2-Methyl-propan-2-ol	1.064867e+0	-6.574171e-4	-1.418512e-6	2.319110e-9	2.181862e-5
Pentan-1-ol	3.021387e+0	-1.835342e-2	5.351012e-5	-5.614921e-8	1.295685e-5
2-Methyl-butan-1-ol	3.094242e+0	-1.912077e-2	5.629933e-5	-5.953733e-8	1.753138e-5
3-Methyl-butan-1-ol	3.197589e+0	-2.011280e-2	5.934238e-5	-6.265298e-8	2.523477e-5
Phenylmethanol	4.044788e+0	-2.567356e-2	7.618533e-5	-7.981666e-8	3.275751e-5
	$u/(ms^{-1})$				
	A_0	A_1	A_2	A_3	σ
Methanol	2073.2354+0	-3.236821	-3.833258e-5	4.225384e-8	7.709652e-4
Ethanol	2.048943e+3	654.9917e-3	-21.77229e-3	32.25250e-6	4.670479e-2
Propan-1-ol	2.342690e+3	-1.798448e+0	-13.74077e-3	23.47478e-6	4.449421e-2
Propan-2-ol	1.284528e+3	7.890793e+0	-44.76469e-3	55.91727e-6	4.678516e-2
Butan-1-ol	22.02576e+3	-190.7489e+0	590.6030e-3	-620.7809e-6	524.0590e-3
Butan-2-ol	2.158110e+3	-292.8004e-3	-16.73948e-3	23.74791e-6	42.90800e-3
2-Methyl-propan-1-ol	4.431432e+3	-21.93397e+0	50.92426e-3	-45.95423e-6	115.2720e-3
2-Methyl-propan-2-ol	2.526164e+3	-3.757354e+0	-6.502289e-3	13.46856e-6	63.12700e-3
Pentan-1-ol	2.482160e+3	-2.418925e+0	-11.84030e-3	21.57812e-6	47.44700e-3
2-Methyl-butan-1-ol	6.203066e+3	-38.88538e+0	106.3147e-3	-106.1553e-6	83.12700e-3
3-Methyl-butan-1-ol	3.141432e+3	-9.188159e+0	10.14029e-3	-2.243478e-6	51.59100e-3
Phenylmethanol	6.308926e+3	-36.37823e+0	94.89900e-3	-89.64920e-6	176.9960e-3

Table 3 Acoustic parameters for the alcohols at 298.15 K.

Table 4 Open literature critical values [82].

	P_c(bar)	T_c(K)	Z_c	ω
Methanol	80.84	512.5	0.222	0.56583
Ethanol	61.37	514.0	0.241	0.64356
Propan-1-ol	51.69	536.8	0.252	0.62043
Propan-2-ol	47.64	508.3	0.250	0.66687
Butan-1-ol	44.14	563.0	0.258	0.58946
Butan-2-ol	42.02	536.2	0.254	0.57678
2-Methyl-propan-1-ol	42.95	548.8	0.258	0.58571
2-Methyl-propan-2-ol	39.72	506.2	0.260	0.61520
Pentan-1-ol	38.97	588.1	0.260	0.57314
2-Methyl-butan-1-ol	39.4	575.4	0.269	0.57362
3-Methyl-butan-1-ol	39.3	577.2	0.268	0.58903
Phenylmethanol	45.5	720.15	0.255	0.36745

where u_∞ is taken as 1600 ms^{-1}, K is a temperature dependent constant ($K = (93.875 + 0.375 \cdot T) \cdot 10^{-8}$), and R and Π are common universal constants (8.3145 $Jmol^{-1}K^{-1}$ and 3.141596, respectively). The values of these parameters, useful for application into calculations of the Collision Factor and Free Length theories, are enclosed in Table 3 for 298.15 K. The evolution of the parameters, intermolecular free length, collision factor and specific acoustic impedance versus temperature are gathered into Figures 5-7.

As observed, intermolecular free length increases with temperature which is coincident with the expansive trend of these compounds and, as noted, their important diminution of density values for rising temperatures. This fact is also evident in terms of collision factor, which shows a clear decreasing trend as a function of temperature. Specific acoustic impedance is a measure of the opposition that a compound presents to the acoustic flow resulting of an acoustic pressure applied to the system, thus is a quantity which depends on the molecular packing of the compound. The decreasing values of the specific acoustic impedance as a function of temperature are in accordance with the presence of progressively weaker interactions among alcohol molecules, as previously commented. The increase of the intermolecular forces is probably the reason for the strong decrease in ultrasonic velocity (Figure 2). Hydrogen bond interactions domain alcohols packing yielding to intense structured net but steric hindrance of the corresponding residual end and individual molecular volume define the intensity of cohesion. As could be expected, attending to the molecular structure of the studied solvents, three different trends should be observed. Firstly, those alcohols showing low molar mass and short residuals gather low values of both measured properties, thus high values of intermolecular free length and low values of collision factor and specific acoustic impedance is observed. Second, molecules of intermediate molar mass or branched residual structure show higher values of density and ultrasonic velocity which, as expected, produces higher values of intermolecular free length and lower values of collision factor and specific acoustic impedance. Third, as an exception phenylmethanol shows the highest values of both thermodynamic magnitudes and thus extreme values for the derived properties earlier commented upon. Packing molecular structure depend on two effects: a) main intermolecular forces among molecules into bulk environment and b) molecular packing as a consequence of size and shape of the molecules. As a consequence, due to the nature of molecular interaction in this kind of compound is based on H-bond, the only fact changing intermolecular forces will be geometrical effects. It is well known the effect associated to hydrophobic headgroups near of hydroxilic groups, producing progressively associations by clusters, bridging neighbouring alcohols by H–bonds and closely packed aliphatic groups by disperse forces. This kind of compounds gather common formation of autoassociative long mean life hydrogen bonds and more rigid bulk structures at any specific temperature. Flat geometry residues as occurs into phenylmethanol produce increasingly strong packing and higher H–bonds probability interactions. The presence of an aromatic ring and a clearly separated hydroxyl group though an aliphatic structure smooth the curious behaviour of gathering notably contractive tendency. This fact is turned into lower values of isentropic compressibility, strong low levels of intermolecular free length and then a more rigid structure.

Temperature is a condition that in all these cases deals towards diminution of density and ultrasonic velocity, probably due to an increasing difficulty of accommodation of the aliphatic end.

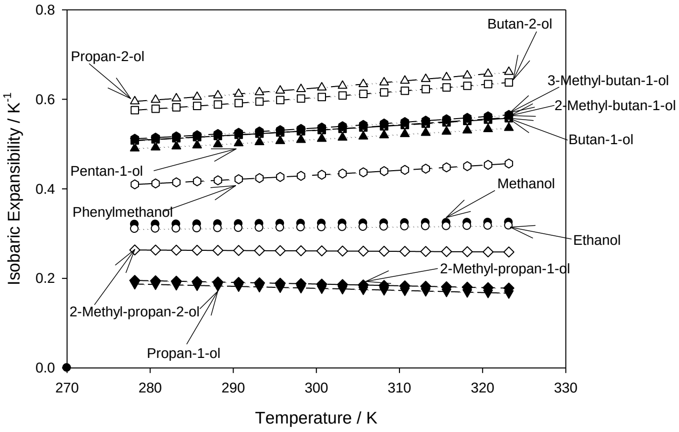

Figure 4. Experimental isobaric expansibility as a function of temperature: (●) methanol, (○) ethanol, (▼) propan-1-ol, (△) propan-2-ol, (■) butan-1-ol, (□) butan-2-ol (◆) 2-methyl-propan-1-ol, (◇) 2-methyl-propan-2-ol, (▲) pentan-1-ol, (▽) 2-methyl-butan-1-ol, (⬢) 3-methyl-butan-1-ol, (⬡) phenylmethanol.

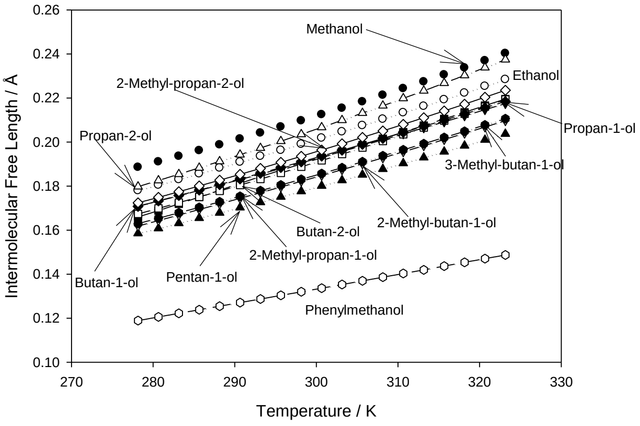

Figure 5. Intermolecular free length as a function of temperature: (●) methanol, (○) ethanol, (▼) propan-1-ol, (△) propan-2-ol, (■) butan-1-ol, (□) butan-2-ol (◆) 2-methyl-propan-1-ol, (◇) 2-methyl-propan-2-ol, (▲) pentan-1-ol, (▽) 2-methyl-butan-1-ol, (⬢) 3-methyl-butan-1-ol, (⬡) phenylmethanol.

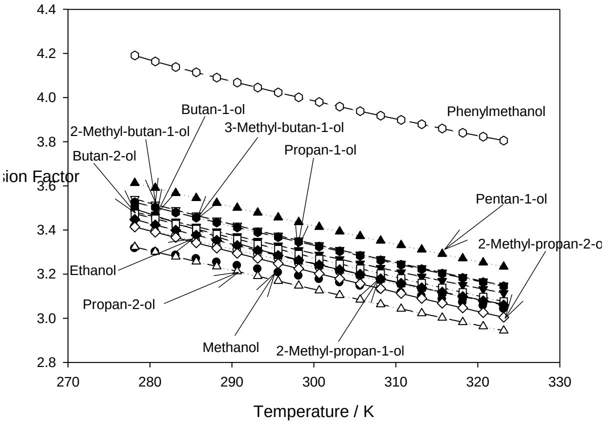

Figure 6. Collision factor as a function of temperature: (●) methanol, (○) ethanol, (▼) propan-1-ol, (△) propan-2-ol, (■) butan-1-ol, (□) butan-2-ol (◆) 2-methyl-propan-1-ol, (◇) 2-methyl-propan-2-ol, (▲) pentan-1-ol, (▽) 2-methyl-butan-1-ol, (⬢) 3-methyl-butan-1-ol, (⬡) phenylmethanol.

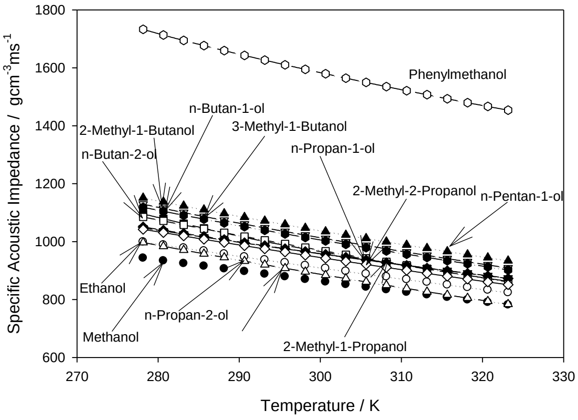

Figure 7. Specific acoustic impedance as a function of temperature: (●) methanol, (○) ethanol, (▼) propan-1-ol, (△) propan-2-ol, (■) butan-1-ol, (□) butan-2-ol (◆) 2-methyl-propan-1-ol, (◇) 2-methyl-propan-2-ol, (▲) pentan-1-ol, (▽) 2-methyl-butan-1-ol, (⬢) 3-methyl-butan-1-ol, (⬡) phenylmethanol.

3.2 Estimation of density

Increasingly, modern process design involves the use of computer aided process design procedures. The physical property packages used in chemical simulators typically rely on generalized equations for predicting properties as a function of temperature, pressure, etc. Despite the success developing several procedures of density estimation for pure compounds or mixtures, only a few of them may be of real application for chemicals of non-ideal trend or high molar mass. An important criteria for estimating the density of these substances, is to understand the complex mechanisms of mixing process, commonly linked to the number and kind of selected “active” molecular groups, and the molecular configuration in terms of 3D structure. Second, the estimation strategy must be account for the strong temperature dependency of density. Both criteria are important for the design of processing facilities and policies that are frequently missing or not taken into account carefully. Perhaps the second criteria is more difficult to develop due to a set of factors are related as branching, molecular flexibility and disperse forces for this kind of compounds which obstruct to translate these facts into an efficient mathematical model.

In this work, different models for density prediction were tested. In this case, a simplification for the Nasrifar–Moshfeghian liquid density correlation (NM correlation) was applied, replacing the Mathias and Copeman temperature-dependent term with the original Soave–Redlich–Kwong equation of state (SRK EOS) temperature-dependent term. This replacement has overcome the limitations in use for the original model which were due to the Mathias and Copeman vapor pressure dependent parameters [51]. The Nasrifar–Moshfeghian model (NM) requires three parameters for each compound, that are not readily available for all compounds. In the absence of these three parameters, the NM correlation fails to predict the density of pure compounds and their mixtures. The modification of this model, Mchaweh–Nasrifar–Moshfeghian model (MNM), overcomes this barrier by replacing the PSRK (Predictive Soave-Redlich-Kwong) parameter α with the original SRK term **(**α_{SRK}). The parameter α_{SRK} is defined in terms of reduced temperature (T_R):

$$\rho / \rho_C = 1 + (1.69 + 0.984 \cdot \omega) / (1 - T_R)^{1/3} + 0.85 \cdot (1 - T_R) \qquad (21)$$

$$\alpha_{SRK} = \left[1 + \dot{m} \cdot \left(1 - \sqrt{T_R}\right)\right]^2 \qquad (14)$$

Where m is given by the following relation as a function of acentric factor (ω):

$$\dot{m} = 0.480 + 1.574 \cdot \omega - 0.176 \cdot \omega^2 \qquad (15)$$

The revised model, after replacement, has the following general formula:

$$\rho = \rho_C \cdot \rho_0 \cdot \left[1 + \delta_{SRK} \cdot \left(\alpha_{SRK} - 1\right)^{1/3}\right] \qquad (16)$$

where ρ_C is the critical density and the parameter δ_{SRK} is a new characteristic parameter for each compound.

$$\delta_{SRK} = 0.1596 \cdot \omega - 0.0319 \qquad (17)$$

The parameter ρ_0 is the reference density and is calculated by the following equation:

$$\rho_0 = 1 + 1.1688 \cdot \left(1 - \frac{T_R}{\alpha_{SRK}}\right)^{1/3} + 1.8177 \cdot \left(1 - \frac{T_R}{\alpha_{SRK}}\right)^{2/3} - 2.6581 \cdot \left(1 - \frac{T_R}{\alpha_{SRK}}\right)^{3/3} + 2.1613 \cdot \left(1 - \frac{T_R}{\alpha_{SRK}}\right)^{4/3} \qquad (18)$$

The critical properties and acentric factors required were found by means open data base [82] as gathered into Table 4.

Rackett and modified Rackett equations of state, are in accordance with the following general expression:

$$\rho = \left(\frac{M \cdot P_C}{R \cdot T_C}\right) \cdot \beta^{\left[1 + (1 - T_R)^{2/7}\right]} \qquad (19)$$

where T_R is the reduced temperature, T_C and P_C are the critical properties of the studied compound, M is the molar mass and β is the critical compressibility factor (Rackett EoS) or an acentric factor dependent parameter which varies attending to a molecular structure parameter (modified Rackett EoS) [52-53].

In order to test the accuracy of different corresponding states methods for the prediction of saturated liquid density of this kind of compounds, we applied the methods proposed by Bradford-Thodos, Riedel, Narsimhan, Yen-Woods, Bhirud and Campbell-Thodos [54-59], in accordance with the following equations:

Bradford-Thodos

$$\rho / \rho_C = 1.0 + (2.924 - 7.34 \cdot Z_C)(1 - T_R) - (1.139 - 3.796 \cdot Z_C)(1 - T_R)^2 + (2.785 - 3.544 \cdot Z_C)(1 - T_R)^{(0.160 + 0.586 Z_C)} \qquad (20)$$

Riedel

$$\rho / \rho_C = 1 + (1.69 + 0.984 \cdot \omega) / (1 - T_R)^{1/3} + 0.85 \cdot (1 - T_R) \qquad (21)$$

Narsimhan

$$\rho / \rho_C = 1 + \left[(0.422 \log P_C + 0.981) / (1 - T_b / T_C)^{0.40}\right] \cdot (1 - T_R)^{0.40} \qquad (22)$$

Yen-Woods

$$\rho / \rho_C = 1 + A(1 - T_r)^{1/3} + B(1 - T_r)^{2/3} + C(1 - T_r)^{4/3} \qquad (23)$$

where

$A = 17.4425 - 214.578 \cdot Z_C + 989.625 \cdot Z_C^2 - 1522.06 \cdot Z_C^3$

If $Z_C \leq 0.26$

$B = -3.28257 + 13.6377 \cdot Z_C + 107.4844 \cdot Z_C^2 - 384.211 \cdot Z_C^3$ If $Z_C > 0.26$

$B = 60.2091 - 402.063 \cdot Z_C + 501.0 \cdot Z_C^2 + 641.0 \cdot Z_C^3$

$C = 0.93 - B$

Bhirud

$$\rho = M \cdot P_c / R \cdot T \cdot \exp(V_0 + \varpi \cdot V_1) \qquad (24)$$

where

$$V_0 = 1.39644 - 24.076 \cdot (T/T_C) + 102.615 \cdot (T/T_C)^2 - 255.719 \cdot (T/T_C)^3 + 355.805 \cdot (T/T_C)^4 - 256.671 \cdot (T/T_C)^5 + 75.1088 \cdot (T/T_C)^6$$

$$V_1 = 13.4412 - 135.7437 \cdot (T/T_C) + 533.38 \cdot (T/T_C)^2 - 1091.453 \cdot (T/T_C)^3 + 1231.43 \cdot (T/T_C)^4 - 728.227 \cdot (T/T_C)^5 + 176.737 \cdot (T/T_C)^6$$

Campbell-Thodos is a model based on Rackett equation (Eq. 19), in which the adjustable parameter β can be expressed as a linear function of (1 – T_R), as follows:

$$\beta = a + b \cdot (1 - T_R) \qquad (25)$$

For polar compounds containing a hydroxyl group:

$$a = [0.690 \cdot T_{Rb} - 0.3342 + (5.79 \cdot 10^{-10} / T_{Rb}{}^{32.75})] \cdot P_C^{0.145}$$

$$b = 0.00318 \cdot s - 0.0211 + 0.625 \cdot \Lambda^{1.35} - 5.90 \cdot \Theta^{0.835}$$

$$\Lambda = P_C^{1/3} / (M^{1/2} \cdot T^{5/6})$$

where Θ is the reduced dipole moment and T_{Rb} is the reduced boiling temperature. The root mean square deviations (eq. 2) between experimental and estimated data are shown in the Table 5. A good agreement (percentage error ≤ 2%) is observed, appearing the lower deviations for Narsimhan, Yen-Woods, Bradford-Thodos and Rackett equations at higher temperatures for all studied alcohols. In general terms, Butan-1-ol, Butan-2-ol, 2-Methyl-propan-1-ol, Propan-2-ol and Pentan-1-ol gather the best results (Figure 8).

Table 5 Root mean square deviations (Eq. 2) for predictive density values by Bradford-Thodos (BT), Riedel (Ri), Narsimhan (N), Yen-Woods (YW), Rackett (R), modified Rackett by Spencer and Danner (mR), Bhirud (B), Campbell-Thodos (CT) and the simplified Nasrifar and Moshfeghian (NMN) models with respect to corresponding experimental data at 278.15 – 323.15 K.

Alcohol	Bradford -Thodos	Riedel	Narsimhan	Yen-Woods	Rackett	Rackett-Spencer-Danner		Bhirud	Campbell-Thodos	MNM
						*	**			
Methanol	0.04557	0.04432	0.01798	0.01742	0.09740	0.05813	0.02208	0.03981	0.02921	0.04447
Ethanol	0.01621	0.06129	0.01941	0.01590	0.04431	0.02837	0.08833	0.02532	0.01879	0.06139
Propan-1-ol	0.00589	0.06535	0.01973	0.01060	0.02406	0.06782	0.12544	0.09670	0.02375	0.06334
Propan-2-ol	0.00611	0.05828	0.00950	0.00317	0.01443	0.05753	0.12595	0.09361	0.04137	0.05895
Butan-1-ol	0.01334	0.05116	0.00386	0.00980	0.00318	0.07103	0.12126	0.09552	0.04619	0.04782
Butan-2-ol	0.00541	0.04962	0.00504	0.00236	0.01254	0.05388	0.09937	0.07616	0.03547	0.05006
2-Methyl-propan-1-ol	0.01996	0.04271	0.00444	0.01627	0.00702	0.06161	0.11004	0.08522	0.04590	0.04104
2-Methyl-propan-2-ol	0.05070	0.01774	0.02885	0.04787	0.04023	0.04464	0.09896	0.07289	0.02221	0.01996
Pentan-1-ol	0.01930	0.04807	0.00918	0.01747	0.00853	0.07310	0.12001	0.09601	0.05274	0.04533
2-Methyl-butan-1-ol	0.04189	0.03871	0.01365	0.05068	0.03646	0.09371	0.14186	0.11700	0.07176	0.03518
3-Methyl-butan-1-ol	0.03663	0.04559	0.01033	0.04369	0.03051	0.09944	0.15179	0.12508	0.05704	0.04371
Phenylmethanol	0.03176	0.01345	0.04868	0.02813	0.01036	0.04146	0.03092	0.03311	0.40696	0.02472

*Considering $\beta = 0.2908-0.099\omega+0.04\omega^2$ **Considering $\beta = 0.29056-0.08775\omega$.

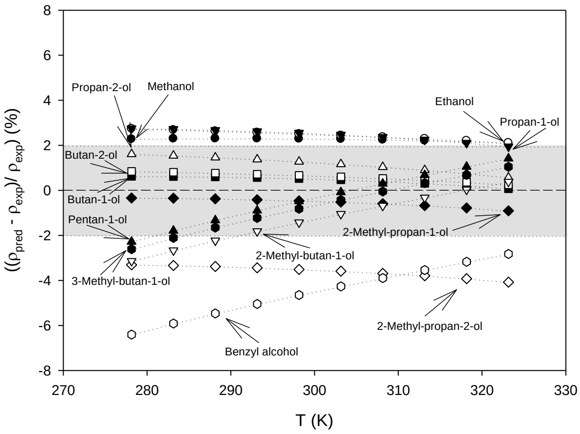

Fig. 8 Density deviation between experimental and predicted data (Nasrihham model) at the temperatures 278.15-323.15 K: (●) methanol, (○) ethanol, (▼) propan-1-ol, (△) propan-2-ol, (■) butan-1-ol, (□) butan-2-ol (◆) 2-methyl-propan-1-ol, (◇) 2-methyl-propan-2-ol, (▲) pentan-1-ol, (▽) 2-methyl-butan-1-ol, (⬢) 3-methyl-butan-1-ol, (⬡) phenylmethanol. The shaded area indicates deviations smaller than 2%.

3.2 Estimation of Ultrasonic Velocity

Recently, an increasingly interest for the application of low/high frequency ultrasound techniques for thermodynamic applications has occurred. Without doubt it is caused by the versatile uses that these measurements may have as heat capacity, compressibility studies or simple and accurate concentration measurements. Ultrasonic velocity has been systematically measured in the last years but this data are scarce yet for simple compounds or any kind of complex mixtures. Predictive procedures are then of primary interest, the same problems that were observed for density prediction being found.

The Collision Factor Theory (CFT) [60] computes the isentropic compressibility by means of collision factors parameters which are a function of temperature into pure solvent or mixture. This model could be expressed by the following expression:

$$\kappa_S = \rho^{-1} \cdot \left(\frac{u_\infty \cdot S \cdot B}{V} \right)^{-2} \tag{26}$$

where u_∞ is 1600 m/s, S is the collision factor, B is the actual volume of molecule per mole and V is the molar volume.

The pertinent relations for this calculation and it theoretical basis were detailed described in the literature indicated above. The collision factors (S) of the pure solvents used in the CFT calculations were estimated by using the experimental ultrasonic velocities, and the molar volumes enclosed in this paper. The characteristic molar volumes were calculated by the group contribution method of Bondi [83]. The experimental data for the ultrasonic velocities of the chemicals studied here were compared with values determined by this theoretical procedure. The deviations of this procedure for the studied alcohols are gathered in Table 6 using the pure parameters from Table 3 and literature data. As observed, the lowest deviations are obtained for the heavier alcohols (lower than 1%), an overestimation being obtained at any case. As observed, temperature is a secondary factor and slightly affects the final prediction.

Table 6 Root mean square deviations for predictive ultrasonic velocities values by means of Collision Factor Theory with respect to corresponding experimental data for the used chemicals at the range 278.15 – 323.15 K.

component	CFT
Methanol	15.54
Ethanol	13.04
Propan-1-ol	11.46
Propan-2-ol	11.45
Butan-1-ol	10.34
Butan-2-ol	10.34
2-Methyl-propan-1-ol	10.34
2-Methyl-propan-2-ol	10.34
Pentan-1-ol	9.51
2-Methyl-butan-1-ol	9.50
3-Methyl-butan-1-ol	9.50
Phenylmethanol	8.62

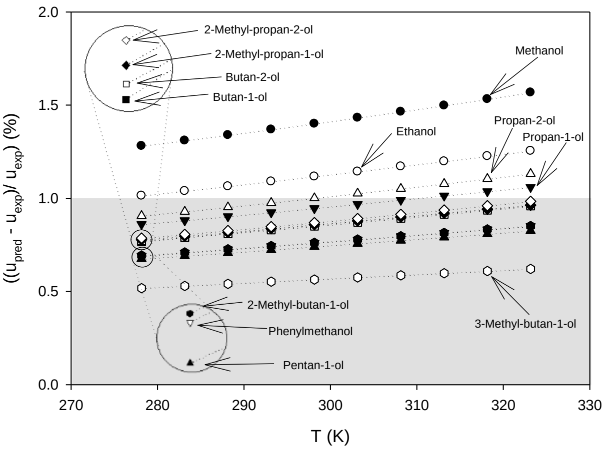

Fig. 9 Ultrasonic velocity deviation between experimental and predicted data (CFT model) at the temperatures 278.15- 323.15 K: : (●) methanol, (○) ethanol, (▼) propan-1-ol, (△) propan-2-ol, (■) butan-1-ol, (□) butan-2-ol (◆) 2-methyl-propan-1-ol, (◇) 2-methyl-propan-2-ol, (▲) pentan-1-ol, (▽) 2-methyl-butan-1-ol, (⬢) 3-methyl-butan-1-ol, (⬡) phenylmethanol. The shaded area indicates deviations smaller than 1%.

4. Comparison with Open Literature Data

Different collections of density or ultrasonic velocity data are disposable into open literature [84-164]. Despite this fact, valuable collections of accurate data, as well as, information as a function of temperature into a wide range are really scarce. Many times, it is no easy to identify the final quality of the data because the purification process of the solvents, the devices calibration or the accuracy of the measurements is not commented upon. As expected, information related to ultrasonic measurements is really more dispersed and scarce. Figures 10-21 and Figures 22-33 show comparison between disposable open information of density and ultrasonic velocity data, respectively, for the studied alcohols as a function of temperature. All these figures gather a zero deviation line which show coincidence between our data and the corresponding earlier published data. As above pointed out, many collection only contribute with an individual point or a few data at different temperatures. Wide range collections are scarce.

In general terms, an adequate agreement with previously published data is observed. For each alcohol should be found a few collection of poor quality an anomalous trend in density ([91] for methanol; [102] for ethanol; [78, 95, 102, 111] for propan-1-ol; [95,111,121] for butan-1-ol; [109] for 2-methyl-propan-1-ol and for 2-methyl-propan-2-ol; [112,144] for pentan-1-ol) and in ultrasonic velocity ([95,98] for methanol; [78] for butan-1-ol; [109;124] for butan-2-ol; [109] for 2-methyl-propan-1-ol; [109] for 2-methyl-propan-2-ol).

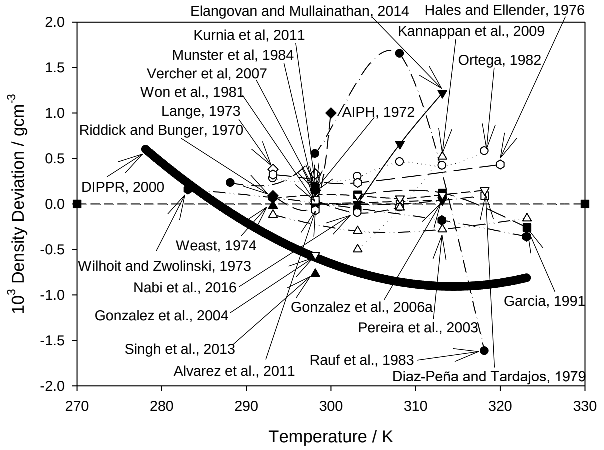

Fig. 10 Density deviations between the experimental data and open literature data for methanol:
(▽,— —, AIPH, 1972), (⬢,— · · —, Wilhoit and Zwolinski, 1973), (◇, Lange, 1973), (▲, Weast, 1974), (⬡,——, Hales and Ellender, 1976), (□,— · —, Diaz-Peña and Tardajos, 1979), (□, Won et al., 1981), (○,···, Ortega, 1982), (●,— · —, Rauf et al., 1983), (◆, Munster et al., 1984), (◆,— —, Riddick et al., 1986), (■, ——, Garcia, 1991), (●, DIPPR, 2000), (△,— · · —, Pereira et al., 2003), (▽, Gonzalez et al., 2004), (▼,——, Gonzalez et al., 2006b), (◆, Vercher et al., 2007), (△,···, Kannappan et al., 2009), (⬡, Alvarez et al., 2011), (⬢, Kurnia et al., 2011), (▲, Singh et al., 2013), (▼,——, Elangovan and Mullainathan, 2014), (○,— —, Nabi et al., 2016).

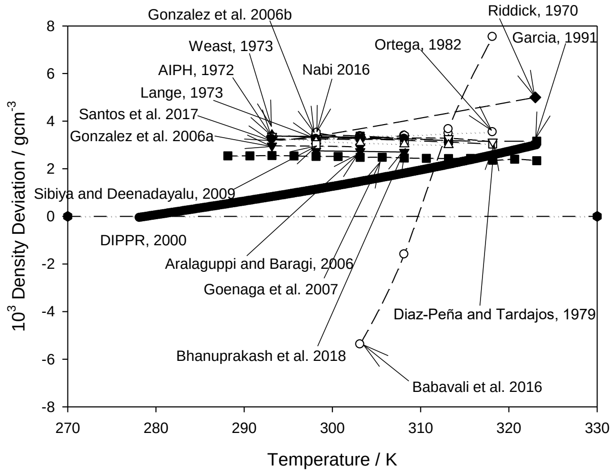

Fig. 11 Density deviations between the experimental data and open literature data for ethanol: (▽,— —, AIPH, 1972), (◇, Lange 1973), (▲, Weast, 1974), (⬡,——, Hales and Ellender, 1976), (□,— · —, Diaz-Peña and Tardajos 1979), (○,···, Ortega, 1982), (●,— · —, Rauf et al., 1983), (■,——, Garcia, 1991), (●, DIPPR, 2000), (△,— · · —, Pereira, 2003), (▼,— —, Gonzalez et al., 2006a), (△,— · · —, Gonza[lez et al., 2006b), (■, Goenaga et al., 2007), (□, Sibiya and Deenadayalu, 2009), (△,···, Kannappan et al., 2009), (▼,——, Elangovan and Mullainathan, 2014), (▼,——, Aralaguppi and Baragi, 2006), (○,— —, Babavali et al., 2016), (○,— —, Nabi et al., 2016) (●,— · —, Santos et al., 2017), (◆,— —, Riddick et al., 1986).

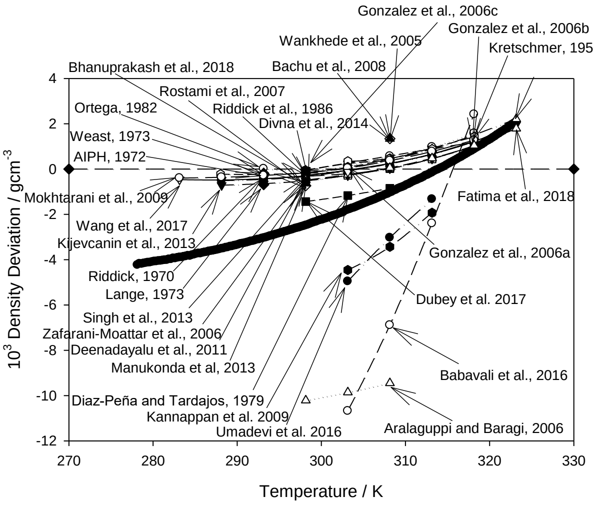

Fig. 12 Density deviations between the experimental data and open literature data for propan-1-ol:
(⬡,— —, Kretschmer, 1951), (□,— · —, Riddick, 1970), (▲, AIPH, 1972), (◆, Lange, 1973), (◇, Weast, 1974), (■,— —, Diaz-Peña and Tardajos, 1979), (○,···, Ortega, 1982), (▲, Riddick et al., 1986), (△,— · · —, Garcia, 1991), (●, DIPPR, 2000), (▲,Wankhede et al., 2005), (⬢,···, Gonzalez et al., 2006a), (▼,— —, Gonzalez et al., 2006b), (●,— —, Gonzalez et al., 2006c), (△,···, Aralaguppi and Baragi, 2006), (□, Zafarani-Moattar et al., 2006), (◇, Rostami et al., 2007), (◇, Bachu et al., 2008), (⬢,— · · —, Kannappan et al., 2009), (○,— —, Mokhtarani et al., 2009), (◆, Deenadayalu et al., 2011), (▼,— · —, Kijevcanin et al., 2013), (▽,— · —, Manukonda et al., 2013), (■, Singh et al., 2013), (●,— · · —, Divna et al., 2014), (●,— · —, Umadevi et al., 2016), (○,— —, Babavali et al., 2016), (■, — —, Dubey et al., 2017), (▽,— —, Wang et al., 2017), (□,— · · —, Bhanuprakash et al., 2018), (□,— —, Fatima et al., 2018).

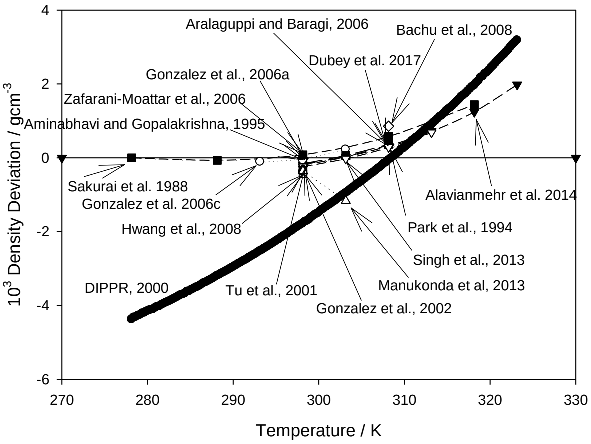

Fig. 13 Density deviations between the experimental data and open literature data for propan-2-ol: (■,---, Sakurai et al., 1988), (▲, Park et al., 1994), (◇,——, Aminabhavi and Gopalakrishna, 1995), (●, DIPPR, 2000), (⬢, Tu et al., 2001), (●, Gonzalez et al., 2002), (△,— · · —, Aralaguppi and Baragi, 2006), (○, Gonzalez et al., 2006a), (○,···, Gonzalez et al., 2006c), (⬡, Zafarani-Moattar et al., 2006), (◇, Bachu et al., 2008), (◆, — —, Hwang et al., 2008), (△,···, Manukonda et al., 2013), (▽,— —, Singh et al., 2013), (▼,---, Alavianmehr et al., 2016), (■, — —, Dubey et al., 2017).

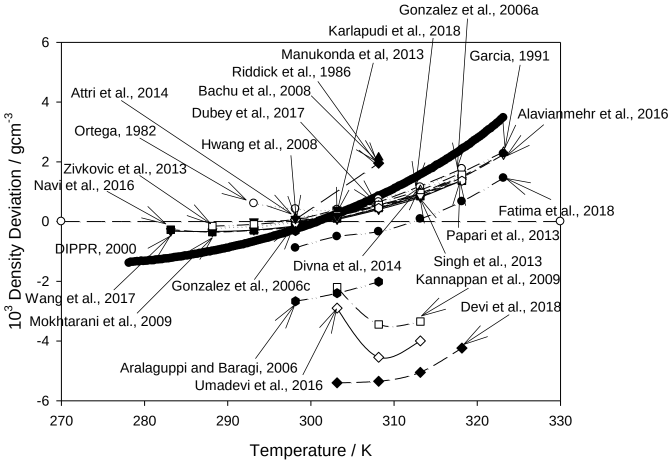

Fig. 14 Density deviations between the experimental data and open literature data for butan-1-ol:
(○,···, Ortega 1982), (◆,— —, Riddick et al., 1986), (△,— · · —, Garcia 1991), (●, DIPPR, 2000), (⬢,— · · —, Aralaguppi and Baragi, 2006), (▼,- - -, Gonzalez et al. 2006a), (⬢,···, Gonzalez et al., 2006c), (▲,— —, Bachu et al., 2008), (◇,— · —, Hwang et al., 2008), (□,— · —, Kannappan et al., 2009), (■,- - -, Mokhtarani et al., 2009), (▼,— · —, Manukonda et al., 2013), (▽,- - -, Papari et al., 2013), (▽,——, Singh et al., 2013), (□,— · · —, Zivkovic et al., 2013), (▲,···, Attri et al., 2014), (△,···, Divna et al., 2014), (●,— · —, Alavianmehr et al., 2016), (■,— —, Nabi et al., 2016), (◇,——, Umadevi et al., 2016), (⬡, — —, Dubey et al., 2017), (▼,——, Wang et al., 2017), (◆, — —, Devi et al., 2018), (●,— · · —, Fatima et al., 2018), (○,——, Karlapudi et al., 2018).

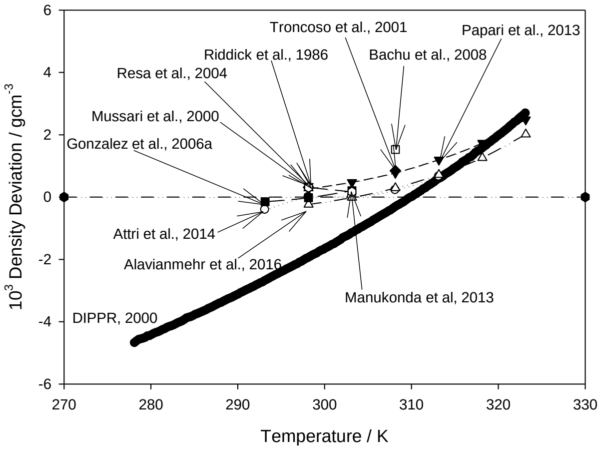

Fig. 15 Density deviations between the experimental data and open literature data for butan-2-ol: (▽,- - -, Riddick et al., 1986), (●, DIPPR 2000), (◇,——, Mussari et al., 2000), (◆, — —, Troncoso et al., 2001), (▲,···, Resa et al., 2004), (■,— —, Gonzalez et al., 2006a), (□,— · —, Bachu et al., 2008), (⬡ ,— —, Manukonda et al., 2013), (▼,- - -, Papari et al., 2013), (○,···, Attri et al., 2014), (△,— · · —, Alavianmehr et al., 2016).

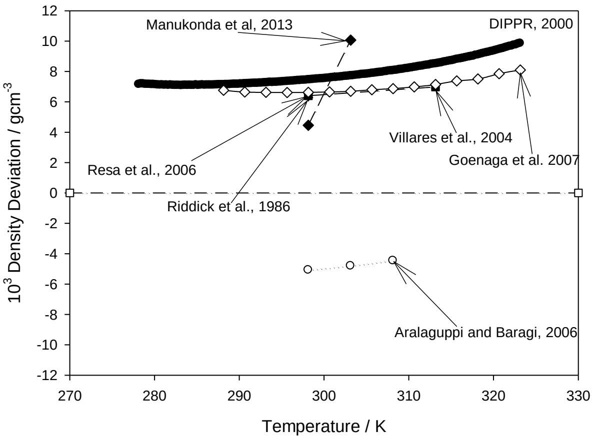

Fig. 16 Density deviations between the experimental data and open literature data for 2-methyl-propan-1-ol: (△,— · · —, Riddick et al., 1986), (●, DIPPR 2000), (▰,— — , Villares et al., 2004), (○,···, Aralaguppi and Baragi, 2006), (▼,- - -, Resa et al., 2006), (◆,— —, Manukonda et al., 2013).

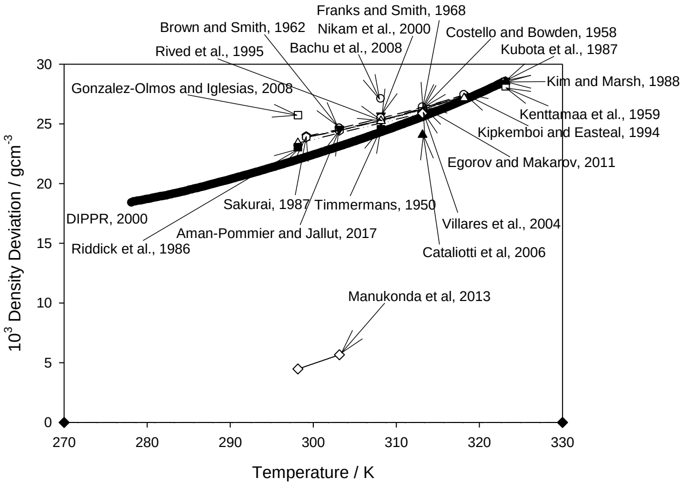

Fig. 17 Density deviations between the experimental data and open literature data for 2-methyl-propan-2-ol: (□, Timmermans, 1965), (▲, Costello and Bowden, 1958), (◆, — —, Kenttamaa et al., 1959), (△, Brown and Smith, 1962), (◇, Franks and Smith, 1968), (▰, Riddick et al., 1986), (▽, Kubota et al., 1987), (▼,——, Kim and Marsh, 1988), (⬢,— · · —, Sakurai, 1988), (▰,- - -, Kipkemboi and Easteal, 1994), (○, Rived et al., 1995), (●, DIPPR 2000), (▼, Nikam et al., 2000), (△,— · · —, Villares et al., 2004), (▲, Cataliotti et al, 2006), (○, Bachu et al., 2008), (□, Gonzalez-Olmos and Iglesias, 2008), (●,— · —, Egorov and Makarov, 2011), (◇,——, Manukonda et al., 2013), (▽,— —, Aman-Pommier and Jallut, 2017).

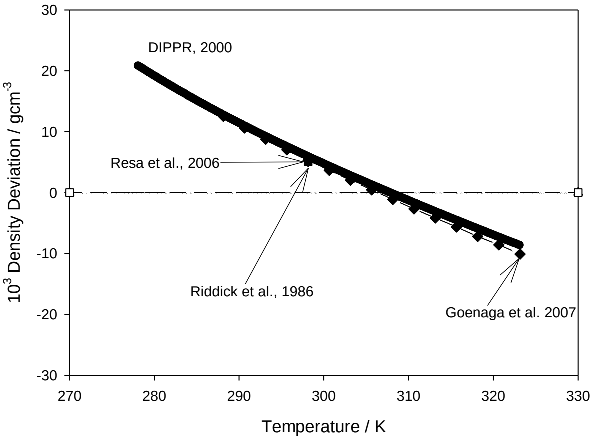

Fig. 18 Density deviations between the experimental data and open literature data for 2-methyl-butan-1-ol: (▼, Riddick et al., 1986), (●, DIPPR 2000), (○, Resa et al., 2006), (◆, Goenaga et al., 2007).

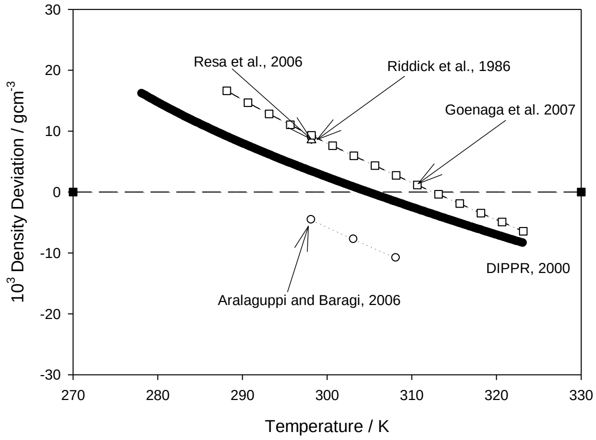

Fig. 19 Density deviations between the experimental data and open literature data for 3-methyl-butan-1-ol: (△, Riddick et al., 1986), (●, DIPPR 2000), (○,···, Aralaguppi and Baragi, 2006), (▼, Resa et al., 2006), (□, Goenaga et al., 2007).

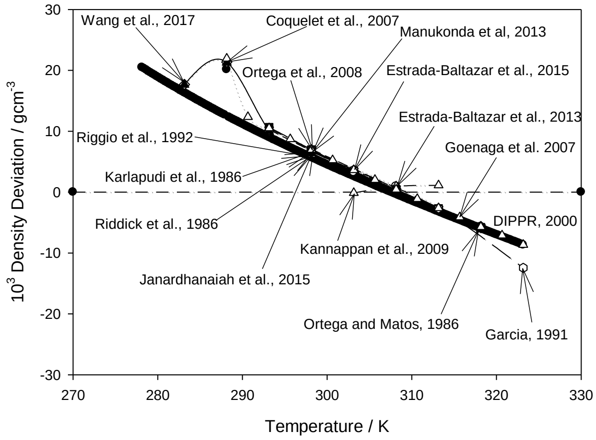

Fig. 20 Density deviations between the experimental data and open literature data for pentan-1-ol: (◆, Ortega and Matos, 1986), (□, Riddick et al., 1986), (▼, Riggio et al., 1992), (●, DIPPR 2000), (▲,···, Coquelet et al., 2007), (△,···, Goenaga et al., 2007), (▰, Ortega et al., 2008), (△,— · · —, Kannappan et al., 2009), (⬢,— · · —, Estrada-Baltazar et al., 2013), (○,— —, Manukonda et al., 2013), (▽,- - -, Estrada-Baltazar et al., 2015), (▼,— —, Janardhanaiah et al., 2015), (◇,——, Wang et al., 2017), (○,···, Karlapudi et al., 2018).

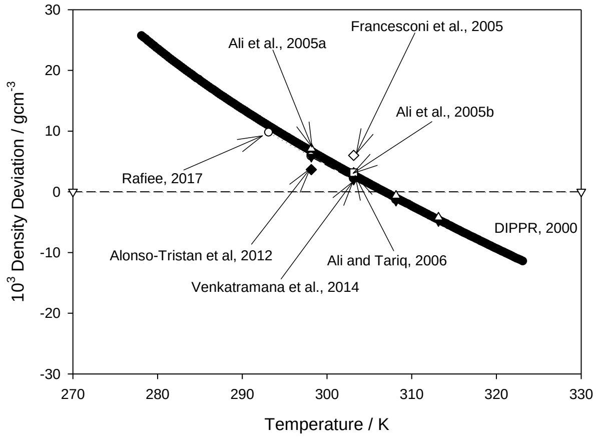

Fig. 21 Density deviations between the experimental data and open literature data for phenylmethanol:

(●, DIPPR 2000), (△,— · · —, Ali et al., 2005a), (□, Ali et al., 2005b), (◇,——, Francesconi et al., 2005), (■, Ali and Tariq, 2006), (◆, Alonso-Tristan et al., 2012), (▼,— —, Venkatramana et al., 2014), (○,···, Rafiee, 2017).

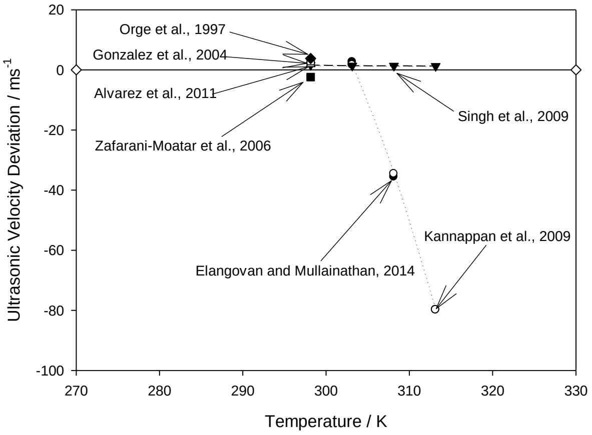

Fig. 22 Ultrasonic velocity deviations between the experimental data and open literature data for methanol: (◆, Orge et al., 1997), (△, Gonzalez et al., 2004), (■, Zafarani-Moatar et al., 2006), (○,···, Kannappan et al., 2009), (▼,- - -, Singh et al., 2009), (□, Alvarez et al., 2011), (●,···, Elangovan and Mullainathan, 2014).

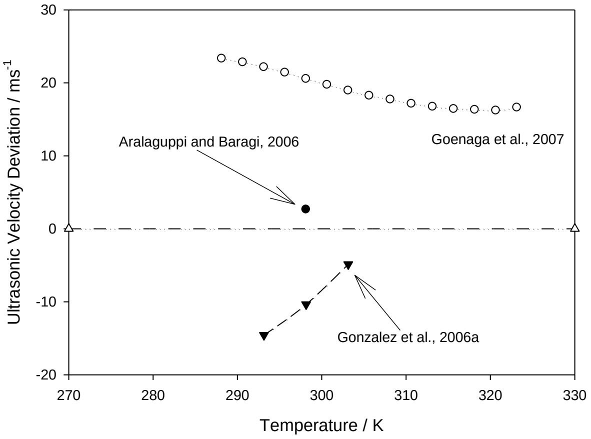

Fig. 23 Ultrasonic velocity deviations between the experimental data and open literature data for ethanol: (●, Aralaguppi and Baragi, 2006), (▼, Gonzalez et al., 2006a), (○, Goenaga et al., 2007).

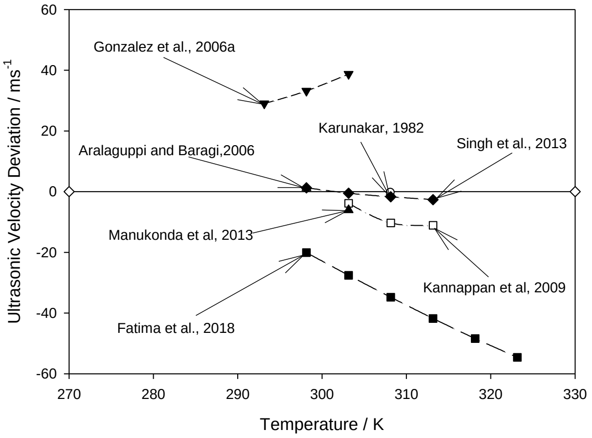

Fig. 24 Ultrasonic velocity deviations between the experimental data and open literature data for propan-1-ol: (○, Karunakar et al, 1982), (△, Aralaguppi and Baragi, 2006), (▼, Gonzalez et al., 2006a), (□, Kannappan et al., 2009), (▲,Manukonda et al., 2013), (◆, Singh et al., 2013), (■, Fatima et al., 2018).

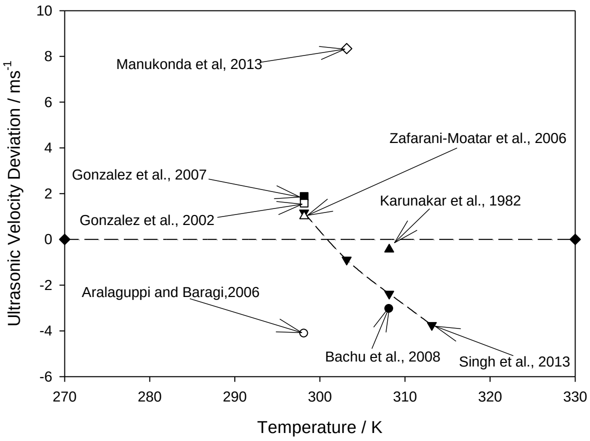

Fig. 25 Ultrasonic velocity deviations between the experimental data and open literature data for propan-2-ol: (▲, Karunakar et al, 1982), (□, Gonzalez et al., 2002), (○, Aralaguppi and Baragi, 2006), (△, Zafarani-Moatar et al., 2006), (■, Gonzalez et al., 2007), (●, Bachu et al., 2008), (◇,Manukonda et al., 2013), (▼, Singh et al., 2013).

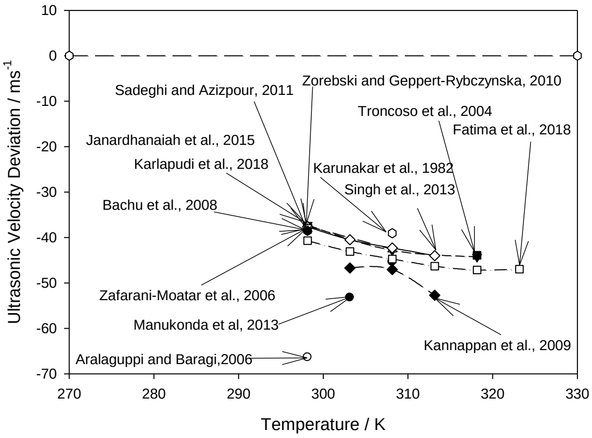

Fig. 26 Ultrasonic velocity deviations between the experimental data and open literature data for butan-1-ol: (⬡, Karunakar et al, 1982), (■, Troncoso et al., 2004), (○, Aralaguppi and Baragi, 2006), (⬢, Zafarani-Moatar et al., 2006), (●, Bachu et al., 2008), (◆, Kannappan et al., 2009), (▽, Zorebski and Geppert-Rybczynska, 2010), (▲,Sadeghi and Azizpour, 2011), (●, Manukonda et al., 2013), (◇, Singh et al., 2013), (△, Janardhanaiah et al., 2015), (□, Fatima et al., 2018), (▼, Karlapudi et al., 2018).

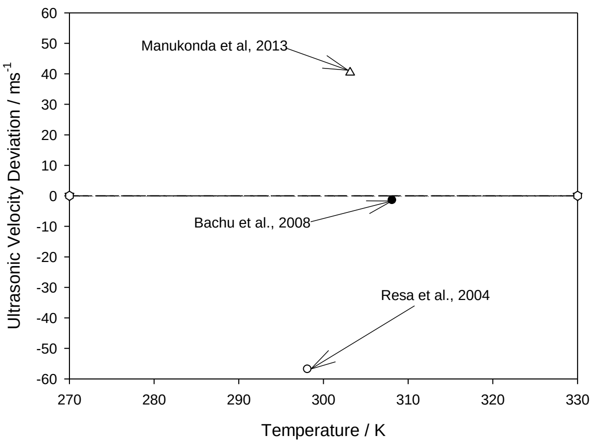

Fig. 27 Ultrasonic velocity deviations between the experimental data and open literature data for butan-2-ol: (○, Resa et al., 2004), (●, Bachu et al., 2008). (△, Manukonda et al., 2013).

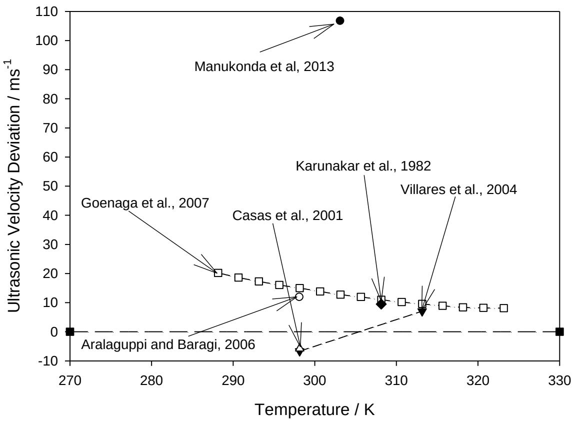

Fig. 28 Ultrasonic velocity deviations between the experimental data and open literature data for 2-methyl-propan-1-ol: (◆, Karunakar et al, 1982), (△, Casas et al., 2001), (▼, Villares et al., 2004), (○, Aralaguppi and Baragi, 2006), (□, Goenaga et al., 2007), (●, Manukonda et al., 2013).

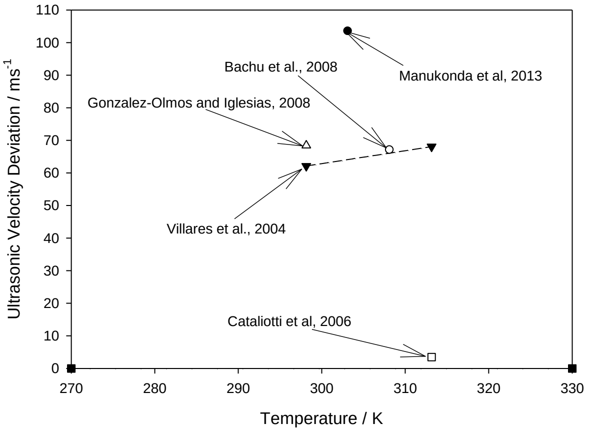

Fig. 29 Ultrasonic velocity deviations between the experimental data and open literature data for 2-methyl-propan-2-ol: (▼, Villares et al., 2004), (□, Cataliotti et al., 2006), (○, Bachu et al., 2008), (△, Gonzalez-Olmos and Iglesias, 2008), (●, Manukonda et al., 2013).

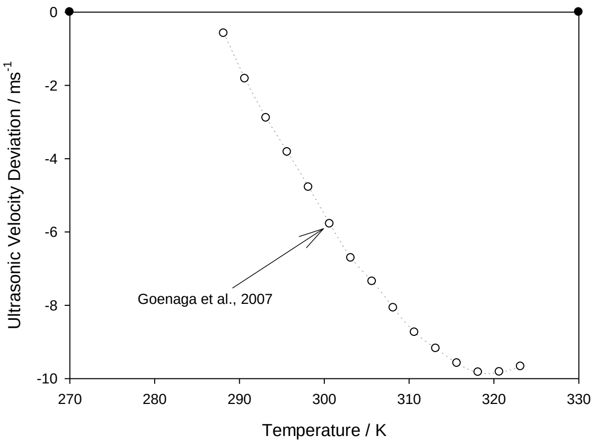

Fig. 30 Ultrasonic velocity deviations between the experimental data and open literature data for 2-methyl-butan-1-ol: (○, Goenaga et al., 2007).

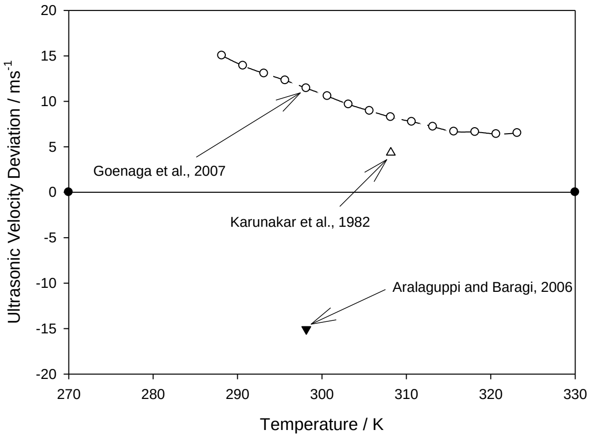

Fig. 31 Ultrasonic velocity deviations between the experimental data and open literature data for 3-methyl-butan-1-ol: (△, Karunakar et al, 1982), (▼, Aralaguppi and Baragi, 2006), (○, Goenaga et al., 2007).

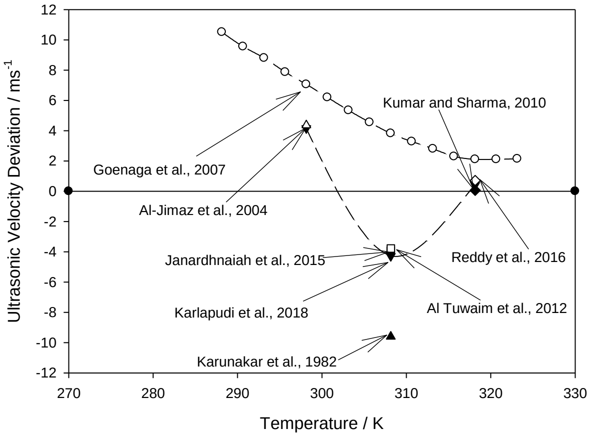

Fig. 32 Ultrasonic velocity deviations between the experimental data and open literature data for pentan-1-ol: (▲, Karunakar et al, 1982), (△, Al-Jimaz et al., 2004), (○, Goenaga et al., 2007), (◆, Kumar and Sharma, 2010), (□, Al Tuwaim et al., 2012), (■, Janardhanaiah et al., 2015), (Reddy et al., 2016), (▼, Karlapudi et al., 2018). .

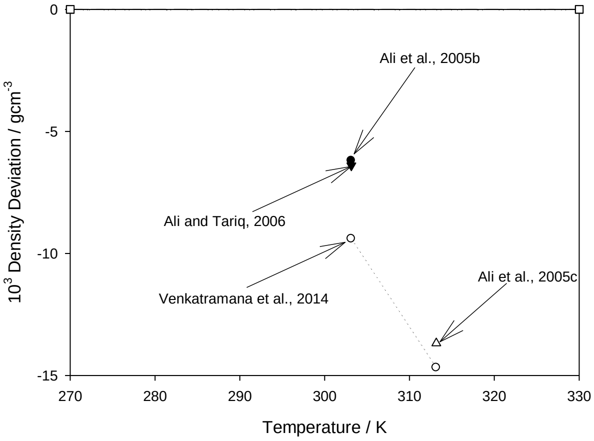

Fig. 33 Ultrasonic velocity deviations between the experimental data and open literature data for phenylmethanol: (●, Ali et al., 2005b), (△, Ali et al., 2005c), (▼, Ali and Tariq, 2006), (○, Venkatramana et al., 2014).

5. Conclusions

It is well known that thermodynamic magnitudes govern the behaviour of mixing chemicals involved into chemical processes. High quality values of basic thermodynamic properties can be applied to model and design industrial devices and transference processes in chemical industry. Density and ultrasonic velocity has been a subject of core interest during the recent past years due to measurements of these magnitudes in solutions formed by liquid components show the degree of deviation from ideality behaviour. These deviations have been used to gain insight into nature and degree of molecula interactions among the enclosed components into the studied systems. Accurate data of density and ultrasonic velocity as a function of composition and temperature/pressure help to understand the nature of the individual chemicals and molecular interactions in complex systems and extreme operational conditions.

In this paper, original data for the temperature dependence of density and ultrasonic velocity at the range of temperature 278.15 - 323.15 K and atmospheric pressure of a collection of alcohols (methanol, ethanol, propan-1-ol, propan-2-ol, butan-1-ol, butan-2-ol, 2-methyl-propan-1-ol, 2-methyl-propan-2-ol, pentan-1-ol, 2-methyl-butan-1-ol, 3-methyl-butan-1-ol, and phenylmethanol) have been measured.

Thermodynamically important parameters giving useful information has also been derived from the experimental physical properties. Isobaric expansibility (α), intermolecular free length (Lf), van der Waals constant (b), molecular radious (r), geometrical volume (B), molar surface area (Y), available volume (Va), volume at absolute zero (V0), molar sound velocity (Ra), collision factor (S) and specific acoustic impedance (Z) were analyzed as a function of temperature.

In what is referred to theoretical estimation, as it could be observed in Figs. 8-9, the better results are showed for the applied models at high temperatures for density, the Nasrimham model offering the best results, and low temperatures for ultrasonic velocity prediction using CFT model. The predictive density equations showed a wide validity range, allowing greater precision (percentage error ≤ 1%), in general terms, for temperatures above 290K. Such equations are partially restricted in the application to high molecular weight alcohols, such as benzyl alcohol and 2-methyl-propan-2-ol, presenting for these deviations greater than 2%, even at high temperatures.

On the other hand, the collision factor theory model has a good predictive capacity over the entire range of temperature studied, without apparent application restrictions. As a whole, the studied models are, at least, of qualitative accuracy in terms of estimation. Deviations yielded for these magnitudes should be considered as a satisfactory result, supporting their validity as predictive tools for the studied alcohols.

Acknowledgments

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