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Speed of sound, density and derivative properties of diisopropyl ether under high pressure

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ABSTRACT

Accurate knowledge of physical and acoustical properties is of importance in many fields of science and engineering. In this work, density and speed of sound measurements of diisopropyl ether (DIPE) are reported. The speed of sound has been measured up to 100 MPa and in the temperature range (293.15–353.15) K by using an apparatus based on a pulse echo technique working in transmission mode, and a correlation for this property was proposed. By using a procedure which rests on the Newton-Laplace relationships, density and its derivatives were determined. To show the reliability of this method, high pressure density measurements were carried out up to 140 MPa and within the temperature interval (293.15–393.15) K with an Anton Paar densitometer.

1. Introduction

Nowadays, industrial applications require environmentally friendly fluids to develop all the processes involving cleaning, refrigeration, solvent extraction, e.g. Ethers play an important role in solvents industry due to its stability, high volatility, and solubility similar to that of the alcohols. Ethers in general are of very low chemical reactivity, and exhibit relatively low boiling points due to they are unable to form hydrogen bonds. Dialkyl ethers as dimethyl ether and diethyl ether are used as solvents while ethyl ether is used too as solvent and as a starter fuel for diesel engines [1]. Tertiary alkyl ethers, as tert-amyl methyl ether (TAME), methyl tert-butyl ether (MTBE), and ethyl tert-butyl ether (ETBE), are being widely used as oxygenate gasoline additives due to its ability to increase the octane number and to raise the oxygen content in gasoline, offering sometimes equal or greater benefits than other commonly used additives such as ethanol.

The use of some of these ethers, as is the case of MTBE, has generated controversy because of its contamination of groundwater [2] and soils, and also due to its toxicity, which have led to search for other substitutes. While ETBE and TAME are still being used due to its favorable environmental properties, diisopropyl ether (DIPE), a dialkyl ether, was introduced as an oxygenate additive for gasolines due to its non-polluting profile [3], and also due to its physical properties, such as the relatively high boiling point [4]. Diisopropyl ether is a secondary ether obtained as a by-product in the production of 2-propanol but a great advantage is that it can be simply produced from the base olefin, propylene and water [5]. Diisopropyl ether has a favorable blending Reid vapor pressure and low solubility in water compared with other ethers, being a good choice as oxygenate gasoline additive. Other uses of diisopropyl ether include solvent for paints, waxes and resins, as solvent in the recovery of phenol in the plastics industry, an extraction agent in metallurgy as it can extract gold from a nitric acid solution. Diisopropyl ether can also be used as solvent in gas chromatography (GC) and in liquid chromatography (LC) analysis.

As diisopropyl ether is a very useful compound in the industry, the availability of reliable scientific data concerning its physical properties as well as its acoustic properties is needed to well develop all the processes involved in the utilization of this compound. High pressure speed of sound measurements in the ranges (0.1–100) MPa for the pressure and (293.15–353.15) K for the temperature have been carried out, broadening the speed of sound data ranges published previously in the literature [6–13]. High pressure density measurements in the ranges (0.1–140) MPa for the pressure and (293.15–393.15) K for the temperature in liquid

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diisopropyl ether were carried out and compared with the literature data available [4,14–21]. An evaluation of the volume and its derivatives has been conducted from an equation of state that represents both the density and the speed of sound.

2. Experimental section

2.1. Materials

Diisopropyl ether, also known as 2,4-dimethyl-3-oxapentane ($C_6H_{14}O$, molar mass: 102.17 g·mol^{-1}, CAS No. 108-20-3), was supplied by Sigma-Aldrich with a mole fraction purity greater than 0.995 certified by gas chromatography by the supplier. The liquid was stored over molecular sieves type 0.4 to avoid any moisture and was used without any further purification except careful degassing before use.

2.2. Speed of sound measurement

High pressure speed of sound data were determined experimentally with a previously described apparatus [22] which consists of an acoustic sensor composed of two piezoelectric transducers facing each other at both ends of a stainless steel cylindrical support and in direct contact with the fluid. The device uses a pulse-echo technique operating at 3 MHz with a fixed path length equal to $L_0 = 30$ mm working in transmission mode to determine the time delay between a transmitted pulse and the first echo of the ultrasonic wave.

The acoustic sensor is fully immersed in the studied liquid within a stainless-steel high-pressure vessel closed at one end by a plug in which three electric feedthroughs were machined.

The temperature inside the cell is regulated thanks to a thermostatic bath and is measured in the liquid by means of a Pt100 probe housed in a metal finger. The uncertainty in temperature measurement is of ±0.1 K. A volumetric pump ensures the compression of the fluid in the whole circuit, being able to reach pressures up to 100 MPa. A pressure gauge capable of measuring up to 100 MPa was used to capture the pressure data. This pressure gauge leads to a pressure measurement with an uncertainty of 0.01 MPa.

As a calibration is needed in order to bring the path length for calculating speed of sound, two reference fluids whose speeds of sounds were measured at different temperatures and pressures were used to this purpose: purified water [23,24] and heptane [25], giving an uncertainty in speed of sound of 0.06%. Taking into account the standard uncertainties in temperature, pressure, the uncertainty in the speed of sound for the calibration and according to the law of propagation of standard uncertainties [26] the expanded uncertainty for the speed of sound in the temperature and pressure ranges measured is estimated to be 0.2%.

2.3. Density measurement

To carry out high pressure density measurements, ρ, in liquid diisopropyl ether, an Anton Paar DMA HPM vibrating tube densitometer connected to a high pressure volumetric pump was used. In such kind of densitometer, the determination of the density is carried out by the measurement of vibration period of the fluid located inside a hollow U-tube. There is a drive element that makes tube vibrate harmonically and a pick-up element for measuring the vibration period [27]. The vibrating tube densitometer utilized allowed us to measure densities in a range of pressures from (0.1–140) MPa every 10 MPa steps with an estimated uncertainty of ±0.015 MPa (Presens Precise Gold Plus pressure transmitter). The temperature measurements were performed in the interval from (293.15–393.15) K. The circulation of a fluid controlled by a thermostatic bath ensures a constant temperature inside the apparatus while a Pt probe located inside the densitometer measures the temperature, giving an uncertainty of ±0.01 K.

Before each campaign of measurements, a calibration was performed according to the procedure described by Comuñas et al. [28] which is a modification of the procedure previously proposed by Lagourette et al. [29]. In this procedure vacuum, and as calibration fluids, water [30] and decane [31] were used due to their known densities. In this way, considering the uncertainties in temperature, in pressure, the uncertainty in measurements of oscillation period, the density of the reference fluids used in the calibration, the overall expanded uncertainty in the experimental density values is estimated to be ±0.5 kg·m^{-3}.

3. Results and discussion

High pressure speed of sound measurements in liquid diisopropyl ether were carried out in the temperature interval (293.15–353.15) K along seven isotherms separated by 10 K for pressures ranging from (0.1–100) MPa every 20 MPa. Due to the low boiling temperature of diisopropyl ether under atmospheric pressure (341.66 K) [32], no measurements were done at 343.15 K and at 353.15 K at atmospheric pressure, avoiding the vapor phase and ensuring all the measurements were done in liquid state. The experimental data of speed of sound for diisopropyl ether can be seen in Table 1. To correlate speed of sound measurements, a rational function with nine adjustable parameters was considered:

$$\frac{1}{c^2} = \frac{A_0 + A_1 T + A_2 T^2 + A_3 T^3 + BP + CP^2 + DP^3}{1 + ET + FP} \quad (1)$$

The values of the nine parameters, together with their deviations (AD%, AAD% and MD%) are included in Table 2. It can be observed in Fig. 1 the comparison between the experimental and calculated speed of sound values from equation (1).

The experimental speed of sound values were compared with data reported in the literature. Seven references report speed of sound data at atmospheric pressure for diisopropyl ether [6–13], and were compared with calculated data by interpolation of our

Table 1
Experimental values of speed of sound, c, at temperatures T and pressures P for diisopropyl Ether.[a]

P/MPa	T/K	c/m·s^{-1}	P/MPa	T/K	c/m·s^{-1}
0.1	293.15	1019.71	60.0	323.15	1278.96
20.0	293.15	1161.24	80.0	323.15	1368.68
40.0	293.15	1274.50	100.0	323.15	1448.65
60.0	293.15	1369.29	0.1	333.15	847.29
80.0	293.15	1454.22	20.0	333.15	1017.78
100.0	293.15	1528.73	40.0	333.15	1146.81
0.1	303.15	974.32	60.0	333.15	1252.38
20.0	303.15	1122.56	80.0	333.15	1343.16
40.0	303.15	1240.38	100.0	333.15	1423.50
60.0	303.15	1337.63	0.1	343.15	
80.0	303.15	1423.43	20.0	343.15	984.53
100.0	303.15	1501.88	40.0	343.15	1117.79
0.1	313.15	930.24	60.0	343.15	1226.40
20.0	313.15	1086.83	80.0	343.15	1318.72
40.0	313.15	1207.91	100.0	343.15	1400.75
60.0	313.15	1308.13	0.1	353.15	
80.0	313.15	1396.71	20.0	353.15	953.14
100.0	313.15	1474.97	40.0	353.15	1090.71
0.1	323.15	887.83	60.0	353.15	1200.36
20.0	323.15	1051.90	80.0	353.15	1294.59
40.0	323.15	1177.10	100.0	353.15	1378.37

[a] Standard uncertainties u are $u(T) = 0.1$ K, $u(P) = 0.01$ MPa. The combined expanded uncertainty U_c (level of confidence = 0.95) is $U_c(c) = 0.002c$.