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Vapour pressures for 1-(butoxymethoxy)butane (dibutoxymethane) and 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxybutane (methyl nonafluorobutyl ether) over the pressure range of (15–80) kPa

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ABSTRACT

Saturated pressures of 1-(butoxymethoxy)butane (dibutoxymethane) and 1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxybutane (methyl nonafluorobutyl ether), new potential solvents for dry-cleaning processes, were measured with a dynamic recirculation apparatus at a pressure range of (15–80) kPa, at temperatures of (390.4–442.7) K for dibutoxymethane and (294.6–322.4) K for methyl nonafluorobutyl ether. The vapour pressures were represented using the correlations of Antoine, extended Antoine and Wagner with relative root mean square deviations of, 1%, 6% and 0.6% for dibutoxymethane, and, 1%, 2% and 0.6% for methyl nonafluorobutyl ether, respectively. The experimental data of dibutoxymethane was compared with those available in literature, the result showed consistency between both data sets.

1. Introduction

There are currently two major washing systems used: (i) Conventional, that uses water as a solvent; and (ii) Dry-cleaning, which uses other than water as a solvent. Despite that conventional washing still has the biggest market share, dry-cleaning still has an important position because it is recommended for natural fibres and delicate clothing. The most efficient and commonly solvent used in the dry-cleaning industry is perchloroethylene (PERC) [1], a volatile organic compound, non-flammable, with a strong characteristic odour. Notwithstanding its efficiency, PERC presents some undesirable side effects, among others, pollutant of groundwater supply [2] and potential responsible of serious human health problems, such as, carcinogenic agent, toxic for liver, kidneys and the central nervous system [3,4]. Carbon dioxide (CO_2), a non-toxic solvent for non-polar solutes used at liquid condition or above its critical point (304.1 K, 7.38 MPa), is an alternative to the dry-cleaning organic solvents. For textile cleaning, CO_2 can remove dirt and easily to be separated from the detergent by depressurization without additional energy [5].

The dry-cleaning industry is constantly looking for new solvents that reduce the impact on the environmental and the human health, and also verified defined physicochemical characteristics needed to design efficient processes. Dibutoxymethane (1-(butoxymethoxy)butane, Fig. 1A) and methyl nonafluorobutyl ether (1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxybutane, Fig. 1B), could be competitive alternatives to PERC. In order to define as appropriated solvents, it is necessary to study and verify harmful effects and physicochemical properties, such as, non-toxicity, inflammability, low ignition point, safe storage and low vaporization of energy value. The search for new solvents with proper characteristics implicate to analyse experimental or realistic modelled data regarding the vapour pressure as a function on temperature of these compounds, information used to estimate the quantity of energy needed for the complete removal of the solvent in the clothing drying phase.

The objective of this work was to contribute with experimental physicochemical values for the vapour pressure in terms of temperature of pure dibutoxymethane and methyl nonafluorobutyl ether, two new potential alternative solvents for dry-cleaning processes, over the pressure range from (15 to 80) kPa. In addition, this study is to provide different alternatives to represent the experimental vapour pressures, such as, correlations of Antoine, extended Antoine, and the Wagner equation.

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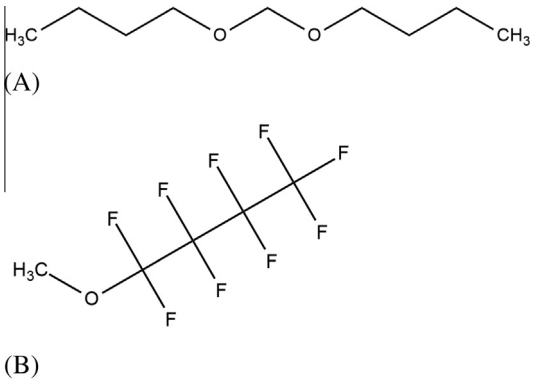

Fig. 1. Chemical structure of (1A) Dibutoxymethane (1-(butoxymethoxy)butane) and (1B) Methyl nonafluorobutyl ether (1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxybutane).

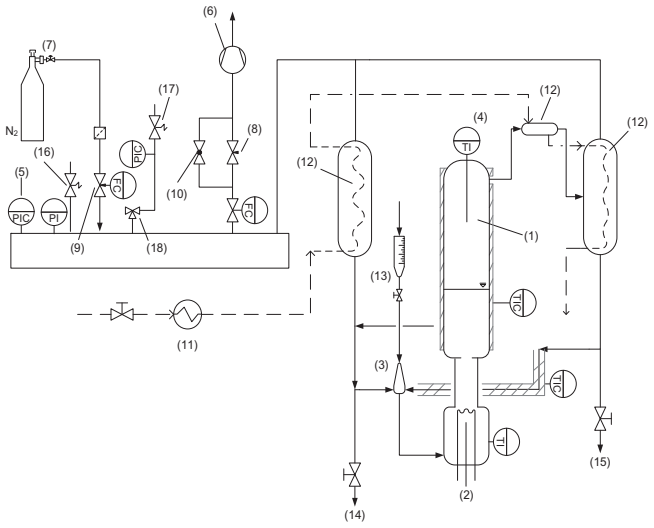

Fig. 2. Experimental apparatus: (1), Cotrell pump; (2), immersion heater; (3), mixing chamber; (4), vapour Pt-100 temperature probe; (5) pressure controller; (6), vacuum pump; (7), N_2 supply; (8), vacuum throttle valve; (9), pressure throttle valve; (10), vacuum by-pass; (11), thermo regulated bath; (12), vapour condensers; (13), filling tunnel; (14) and (15), liquid and vapour samplers; (16), overpressure relief valve; (17), vacuum relief valve; (18), 3/2 way valve.

2. Experimental

2.1. Materials

Dibutoxymethane (1-(butoxymethoxy)butane, >0.99 mass fraction purity, CAS: 2568-90-3) was purchased from Sigma-Aldrich (St. Louis, MO) and methyl nonafluorobutyl ether (1,1,1,2,2,3,3,4,4-nonafluoro-4-methoxybutane, >0.98 mass fraction purity, CAS: 163702-07-6) from AK Scientific (Union City, CA). Reagents were used without further purification. In Table 1, there are summarized specifications of the chemical samples used in this work.

2.2. Apparatus and procedure

The vapour pressure was measured using a commercial all-glass dynamic recirculation isobaric (vapour + liquid) equilibrium (VLE) apparatus (Labodest model 602D, i-Fischer Engineering GmbH, Waldbüttelbrunn, Germany) described by Meneses et al. [6], shown in Fig. 2. Its operation procedure relies on the principle of the recirculation of both liquid and vapour phases at controlled pressure. The advantage of the recirculation method is the rapid appearance of the equilibrium simultaneously with the exact measurement of the boiling temperature. The experimental procedure used was as follows: the pure compound was charged in the apparatus by the filling tunnel (13), the N_2 supply (7) to the system was opened, once the liquid is at the desired level the magnetic stirrer bar was activated (3), the pressure throttle valve (9) is opened, and the vacuum pump (10) was started to work. The desired value of pressure (p) was set on the controller panel, the immersion heater (2) was activated and finally, fine adjustments of pressure were made by manual operation of valve (8). In order to verify that system reached the equilibrium, the temperature (T) stability had to remain constant for a period of time of (15–30) min [7].

The standard uncertainty (u) for temperature and pressure measured were estimated as $u(T) = 0.1$ K and $u(p) = 0.5$ kPa [6]. The expanded uncertainty ($U = k \cdot u$) was calculated with a coverage factor ($k = 2$) multiplier that expand the standard uncertainty up to an specific level of confidence (95.45% in this contribution), resulting $U(T) = 0.2$ K and $U(p) = 1.0$ kPa [8]. Nevertheless, the overall deviation in the values of the vapour pressure, associated to uncertainties of the experimental apparatus and methodology was estimated <0.2%, by direct comparison with measurements of the vapour pressure for n-heptane reported in literature. This value is consistent with results obtained in previous works using the same apparatus and experimental methodology [9].

3. Results and discussion

Experimental temperature and vapour pressure data for dibutoxymethane and methyl nonafluorobutyl are listed in Table 2. For a pressure ranged from (15 to 80) kPa a total of 20 pairs of (T, p) were measured at $390.4\ \text{K} \leqslant T \leqslant 442.7\ \text{K}$ for dibutoxymethane, and 18 pairs at $294.6\ \text{K} \leqslant T \leqslant 322.4\ \text{K}$ for methyl nonafluorobutyl ether. Two functional forms of Wagner equations, (1) and (2) [10], were selected to represent and evaluate the measured vapour pressures.

$$\ln(p^{\text{Calc}}/p_c) = (T_c/T)(c_1 \cdot \tau + c_{1.5} \cdot \tau^{1.5} + c_3 \cdot \tau^3 + c_6 \cdot \tau^6) \quad (1)$$

$$\ln(p^{\text{Calc}}/p_c) = (T_c/T)(c_1 \cdot \tau + c_{1.5} \cdot \tau^{1.5} + c_{2.5} \cdot \tau^{2.5} + c_5 \cdot \tau^5) \quad (2)$$

where p^{Calc} is the calculated vapour pressure, T_c and p_c are the critical temperature and pressure, c_i are the fitting model parameters, and, $\tau = 1 - T/T_c$ is a reversed reduced temperature variable. In Table 3 are listed the critical temperature and pressure as well as

Table 1
Specification of chemical samples.

Chemical name	Source	Initial mass fraction purity/kg·kg^{-1}	Purification method	Final mass fraction purity/kg·kg^{-1}	Analysis method
1-(Butoxymethoxy)butane (dibutoxymethane)	Sigma-Aldrich	0.99	None	0.99	None
1,1,1,2,2,3,3,4,4-Nonafluoro-4-methoxybutane (methyl nonafluorobutyl ether)	AK Scientific	0.98	None	0.98	None