J. Chem. Thermodynamics 53 (2012) 114–118

Contents lists available at SciVerse ScienceDirect

J. Chem. Thermodynamics

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

Supplementary vapor pressure data of the glycol ethers, 1-methoxy-2-propanol, and 2-methoxyethanol at a pressure range of (15 to 177) kPa

Arturo Bejarano [a], Laura J. Poveda [b], Juan C. de la Fuente [a,c,*]

[a] *Departamento de Ingeniería Química y Ambiental, Universidad Técnica Federico Santa María, Avda. España 1680, Valparaíso, Chile*
[b] *Pontificia Universidad Católica (PUC) de Chile, Avda. Vicuña Mackenna 4860, Macul, Santiago, Chile*
[c] *Centro Regional de Estudios en Alimentos Saludables CREAS, Blanco 1623, Valparaíso, Chile*

ARTICLE INFO

Article history:
Received 18 January 2012
Received in revised form 12 April 2012
Accepted 27 April 2012
Available online 8 May 2012

Keywords:
Dynamic recirculation method
Glycol ethers
1-Methoxy-2-propanol
2-Methoxyethanol
Vapor pressure

ABSTRACT

The vapor pressure of pure 1-methoxy-2-propanol and 2-methoxyethanol, commonly used as co-solvents in inks, paints, coatings, organic/water solutions among many other applications, were measured with a dynamic recirculation apparatus at a pressure range of (15 to 177) kPa. The measurements were performed at temperature ranges of (342 to 412) K for 1-methoxy-2-propanol and (346 to 417) K for 2-methoxyethanol. The maximum likelihood method was used to estimate the parameters of the Antoine equation, the parameters of an extended Antoine equation and the Wagner equation were determined by non linear least squares method. The three models showed root mean square deviations (*rmsd*) of 0.39%, 0.38%, and 0.29%, and 0.37%, 0.33%, and 0.32%, for 1-methoxy-2-propanol and 2-methoxyethanol, respectively. Additionally, the experimental data and correlation were compared with those available in the literature.

1. Introduction

Common glycol ethers are oxygenated hydrocarbons of major industrial and economic importance. Since they have both functional hydrophobic and hydrophilic groups they are suitable for a large number of industrial and commercial applications including household products, paints, inks, coatings, cleaning solutions and biochemical applications [1]. Nonetheless, several studies related to toxicity suggest that exposure to glycol ethers (1-methoxy-2-propanol and 2-methoxyethanol, among others) can cause adverse effects on human health [2–5]. Vapor pressure of pure glycol ethers is a relevant property on which the vapor-liquid calculations have a strong dependence and therefore it is of great importance in the design of separation processes. Moreover, several derived physical-chemical properties can be estimated from the vapor pressure data. Besides, limited information regarding vapor pressure data were reported in the literature for the glycol ethers 1-methoxy-2-propanol and 2-methoxyethanol.

The main objective of this work was to contribute with new experimental information of the vapor pressures for the glycol ethers, 1-methoxy-2-propanol and 2-methoxyethanol, in the range of (15 to 177) kPa by measuring the isobaric (vapor + liquid) equilibrium. Additionally, the parameters of three commonly used vapor pressure equations were estimated: the Antoine model, the Wagner model [6], and an extended Antoine model [7].

2. Experimental

2.1. Materials

Pure nitrogen (N_2) was supplied by AGA Chile with no less than 99.999% of N_2. HPLC-grade 2-methoxyethanol and pro-analysis 1-methoxy-2-propanol were obtained from Aldrich (St. Louis, MO) with purity greater than 99.5%. These materials were used without further purification.

2.2. Apparatus and procedures

The vapor pressure was measured using a commercial all-glass dynamic recirculation isobaric (vapor + liquid) equilibrium (VLE) apparatus (Labodest model 602D, *i*-Fischer Engineering GmbH, Waldbüttelbrunn, Germany) [8]. Its operation procedure relies on the principle of the recirculation of both liquid and vapor 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 uncertainty was the uncertainty associated to the equipment which was estimated <0.2%. This estimation was calculated by comparison between the measurements for n-heptane made

---

* Corresponding author at: Departamento de Ingeniería Química y Ambiental, Universidad Técnica Federico Santa María, Avda. España 1680, Valparaíso, Chile. Tel.: +56 32 2654221; fax: +56 32 2654478.

E-mail address: juan.delafuente@usm.cl (J.C. de la Fuente).

0021-9614/$ - see front matter © 2012 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.jct.2012.04.029

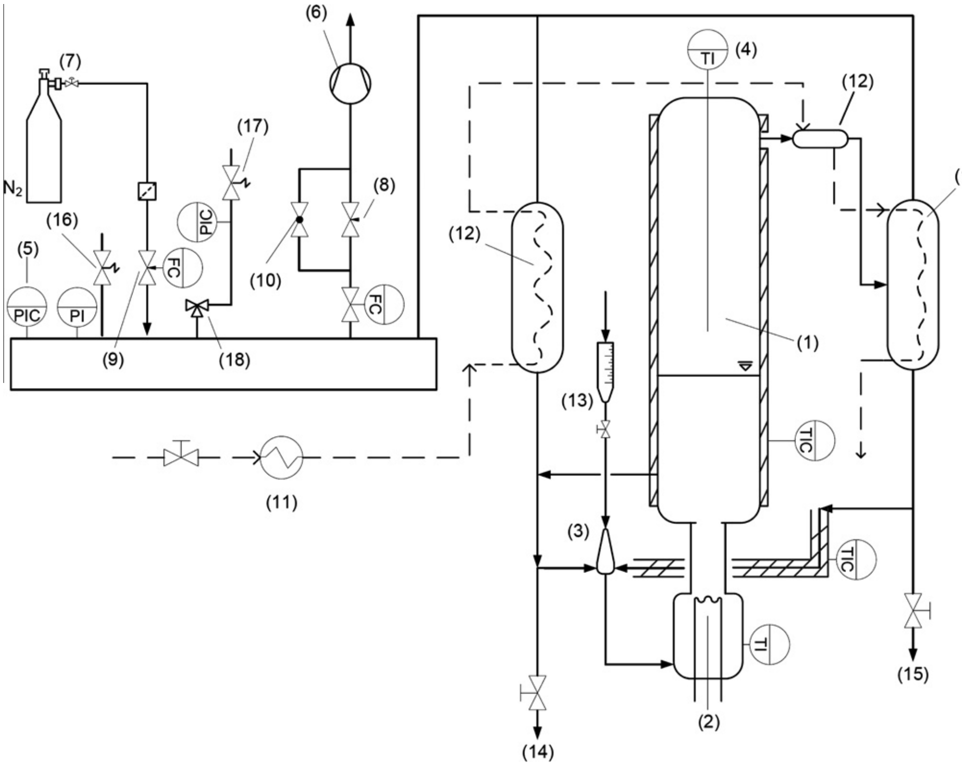

FIGURE 1. Experimental apparatus: (1), Cotrell pump; (2), immersion heater; (3), mixing chamber; (4), vapor Pt-100 temperature probe; (5) pressure controller; (6), vacuum pump; (7), N_2 supply; (8), vacuum throttle valve; (9), pressure throttle valve; (10), vacuum by-pass; (11), thermo regulated bath;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

in our equipment and those reported in literature. The comparison, the apparatus (figure 1) and methodology are described in more detail in our previous work [9]. 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 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 stability had to remain constant (within ±0.1 K) for a period of time of (15 to 30) min [8].

3. Results and discussion

Experimental values of temperature and pressures measured for 1-methoxy-2-propanol at pressure range of (15 to 177) kPa and temperature range of (342 to 412) K and, for 2-methoxyethanol at the same pressure range and temperature range of (346 to 417) K are listed in table 1. The regressed parameters of three vapor pressure equations, described below, along with their root mean square deviation (*rmsd*) are reported in table 2.

The maximum likelihood method was used to estimate the parameters of the Antoine equation (1) in order to take into account its non linear mathematical form and the fact that both temperature and pressure are subject to experimental variability [10].

$$\ln\{p_{\text{cal}}/\text{kPa}\} = A - \frac{B}{T/\text{K} + C} \tag{1}$$

where A, B and C are adjustable parameters. The maximum likelihood objective function to be minimized has the form:

$$S = \sum_i \left[\left(\frac{T - T_{\text{cal}}}{\sigma_{T,i}} \right)^2 + \left(\frac{p - p_{\text{cal}}}{\sigma_{p,i}} \right)^2 \right] \tag{2}$$

where $\sigma_{T,i}$ and $\sigma_{p,i}$ are estimated standard deviations in the measured temperature and pressure for the ith observation. These values were assigned from the experimental set up as $\sigma_{T,i} = 0.1$ K and $\sigma_{p,i} = 0.15$ kPa.

The Wagner equation (3) [7] with four different functional forms, was evaluated to represent the measured vapor pressures.

TABLE 1
Experimental vapor pressures (p) and percent deviations ($10^2 \cdot (p - p_{\text{cal}})/p$) from the Wagner equation (3) for 1-methoxy-2-propanol and 2-methoxyethanol at temperatures T.

1-Methoxy-2-propanol			2-Methoxyethanol		
T/K	p/kPa	$10^2 \cdot (p - p_{\text{cal}})/p$	T/K	p/kPa	$10^2 \cdot (p - p_{\text{cal}})/p$
342.3	15.0	−0.25	346.4	15.0	0.06
352.5	23.5	0.38	356.9	23.5	0.04
360.1	32.0	0.33	364.7	32.0	−0.29
367.4	42.1	−0.24	376.0	49.0	0.07
371.6	49.1	−0.21	380.6	57.5	−0.22
376.0	57.6	0.08	384.5	66.0	0.16
380.0	66.1	−0.09	388.1	74.5	0.19
383.5	74.6	0.26	391.3	83.0	0.50
386.9	83.3	0.04	394.4	91.5	0.28
390.1	92.6	0.27	397.2	100.0	0.34
392.8	99.9	−0.68	400.1	108.5	−0.49
397.9	116.9	−0.68	402.6	117.0	−0.56
400.0	125.5	0.04	404.9	125.5	−0.45
402.2	134.0	0.07	407.0	134.0	−0.11
404.3	142.5	0.08	409.1	142.5	−0.09
406.3	151.0	0.11	411.1	151.0	−0.07
408.2	159.5	0.13	412.9	159.5	0.27
410.0	168.0	0.23	414.7	168.0	0.39
411.8	176.5	0.16	416.6	176.5	0.02