

Measurements of vapor pressure and gaseous pVT property for trans-1,3,3,3-tetrafluoropropene (HFO-1234ze(E))

Jianguo Yin ^{a,*}, Yong Zhou ^b, Guanjia Zhao ^a, Suxia Ma ^a

^a Shanxi Province Key Laboratory of Clean & High Efficient Combustion and Utilization of Circulating Fluidized Bed, Taiyuan University of Technology, Taiyuan, Shanxi, 030024, People's Republic of China

^b Honeywell Integrated Technology (China) Co., Ltd., 430 Libing Road, Zhang Jiang Hi-Tech Park, Pudong New Area, Shanghai, 201203, People's Republic of China

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ABSTRACT

The saturated vapor pressures and gaseous pVT properties for trans-1,3,3,3-tetrafluoropropene (HFO-1234ze(E)) were measured using a Burnett apparatus. For vapor pressure, 15 data points were obtained in the temperature range from (303–373) K and pressure range from (578–3027) kPa. The experimental data was correlated by a Wagner type equation with the average absolute deviation of 0.003%. For gaseous pVT property, 101 data points were obtained in the temperature range from (313–373) K, pressure range from (117–2831) kPa and density range from (0.05–1.6) mol·dm⁻³. The second and third virial coefficients along 13 isotherms were obtained. The density data were correlated by a three-term truncated virial equation of state with a relative standard deviation of 0.06%.

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1. Introduction

HFO-1234ze(E) or trans-1,3,3,3-tetrafluoroprop-1-ene, a fluorinated analogue of propene, is regarded as a promising working fluid in refrigeration and air conditioning system due to its zero ODP (ozone depletion potential), low GWP (global warming potential), low flammability and suitable thermodynamic properties [1,2].

Thermodynamic properties such as saturated vapor pressure and density must be accurately obtained for optimum design and operation of refrigeration system. These properties of HFO-1234ze(E) can be calculated by NIST REFPROP [3] using equations of state compatible with that of Thol and Lemmon [4]. However, the experimental data used for developing the equation of state was few. For vapor pressure, limited open literature were found [5–12], and among them including six for vapor liquid boundary of HFO-1234ze(E) mixtures [13–18]. For vapor phase density, four data sets were found after a literature survey [5,6,19,20].

In this work, vapor pressures and gaseous pVT properties of HFO-1234ze(E) were measured using a Burnett apparatus. A Wagner type vapor pressure equation and a three-term truncated virial

equation of state were developed for the present data and both equations were compared to the literature data.

2. Experimental section

2.1. Materials and methods

The experimental sample of HFO-1234ze(E) was provided by Honeywell with a declared fraction of better than 99.9%. The sample was degassed by freeze-pump-thaw cycle by using liquid nitrogen and a high vacuum pump (<0.001 Pa) for several times. Helium gas was supplied by Taiyuan city An Xuhong cloud Technology Development Co. Ltd. of China with a declared fraction of 99.999%. The chemicals are summarized in Table 1.

The Burnett-isochoric coupling method used in this work to measure the gaseous pVT properties of HFO-1234ze(E) was similar to that of Gupta [21]. Vapor pressures were measured by partially filling the Burnett main cell with liquid and using a static method.

2.2. Apparatus

The schematic diagram of the experimental apparatus is illustrated in Fig. 1. It consists of a Burnett apparatus, a thermostatic

* Corresponding author.

E-mail address: yin.jg@foxmail.com (J. Yin).

Table 1
Chemicals used in this work.

Chemical name	Source	Stated purity	Purification
HFO-1234ze(E)	Honeywell	>0.999	none
Helium	Taiyuan city An Xuhong cloud	0.99999	none

bath, a temperature and pressure measurement system, a sample charging system and a vacuum system.

The Burnett apparatus is composed of two cells: a main cell and an expansion cell. The two cells are all cylinder vessels made of 1Cr18Ni9Ti stainless steel with a wall thickness of more than 20 mm. The inner volume of main cell and expansion cell at room temperature is about 406 cm³ and 196 cm³, respectively. The main cell serves both as the initial sample cell for expansions and the isochoric chamber. The two cells were all polished to reduce the physical adsorption effect. The sample valve (V1), expansion valve (V2) and vacuum valve (V3) were Swagelok non-rotating type valve which could provide excellent seal performance along the whole experimental procedure. The whole apparatus was immersed in a thermostatic bath to establish temperature uniformity and silicone oil was used as a heat transfer medium in the bath. The bath temperature was regulated by a PI controller with the fluctuation of better than ± 5 mK per 30 min.

The temperature measurement system includes a 25 Ω standard platinum resistance thermometer (T25-660-1, ASL) installed near the cells and a digital multimeter (3458A, Agilent). The thermometer was calibrated on the ITS-90 scale at the National Institute of Metrology of China. The combined standard temperature uncertainty was estimated to be less than ± 10 mK in the temperature measurements including the uncertainties of the thermometer, the calibration and the multimeter. The performance of the temperature measurement system was confirmed against the triple point of water before and after the whole experiment. The pressure was measured with a digital quartz pressure transmitter (0–6.9 MPa, 31K-101, Paroscientific) and a differential pressure transducer (3051, Rosemount). The differential pressure transducer was used to separate the sample in the thermostatic bath from nitrogen gas whose pressure was measured by the pressure transmitter outside the bath and its null position was carefully calibrated as a function of temperature before pressure measurements. The pressure transmitter with accuracy of 0.01% full scale stated by the manufacturer was recalibrated against a DHI piston gauge. The accuracy of the transmitter was better than 0.005% full scale after pressure adjustment according to the recalibration results. The overall standard pressure uncertainty was estimated to be less than ± 0.5 kPa, considering the uncertainties of pressure transmitter, piston gauge, differential pressure transducer, the calibration of null position of differential pressure transducer, and pressure fluctuation during measurements.

The high vacuum was provided by a turbo-molecular pump (FD110, KYKY, China, the stated ultimate pressure is 5×10^{-5} Pa).

2.3. Procedure

Before an experiment, all apparatus system was place under vacuum and rinsed with the measured sample for three times, then after the system was discharged to high vacuum again and maintained for at least 12 h, a suitable amount of sample was introduced into the main cell. For pVT properties, HFO-1234ze(E) was charged in the vapor phase. After the desired expansion temperature of the system was reached by means of the thermostatic bath, the valves V1, V4 and V5 were opened and the sample pressure was monitored. Then the sample cylinder and the associated connecting tubing were heated to maintain the sample charging procedure.

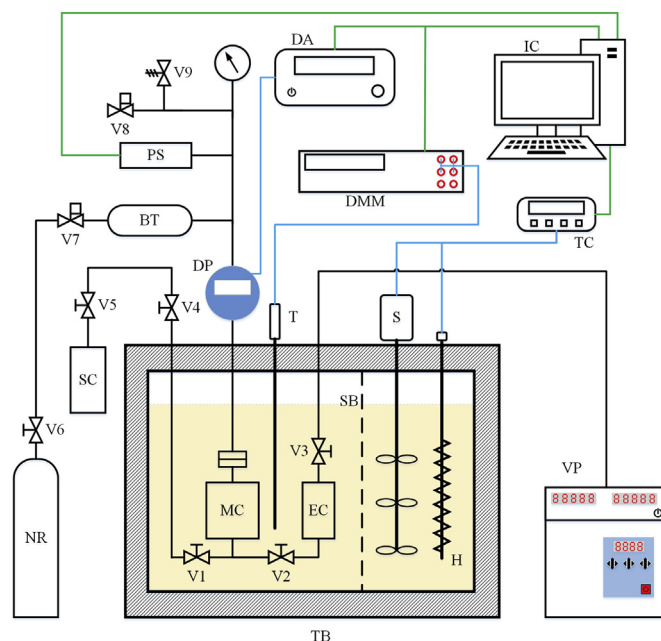


Fig. 1. Schematic diagram of the experimental system: MC: main cell; EC: expansion cell; SB: shield board; S: stirrer; H: heater; TB: thermostatic bath; T: temperature thermometer; DP: differential pressure transducer; NR: nitrogen reservoir; SC: sample cylinder; BT: buffer tank; PS: pressure sensor; DA: digital acquisition; DMM: digital multimeter; TC: temperature controller; IC: industrial computer; VP: high vacuum pump; V1–V3: non-rotating valve; V4–V9: valve.

After the desired sample pressure (a little lower than the saturated pressure at the temperature) was reached, the sample valve V1 was closed and the sequences of thermal equilibrium, temperature and pressure measurement, and temperature change were repeated according to the Burnett-isochoric method to finish the entire p - T surface with a single charge of sample. The temperature and pressure at each state point were recorded for at least 20 min to reduce the experimental error, with the average value of more than 80 measurements used as the final value.

The data of pVT property obtained in this experiment were analyzed by Burnett analysis method along each isotherm. The Burnett analysis method used in this work was similar to that of Stouffer [22]. A truncated virial equation of state used in the regression is expressed as follows:

$$p_i = RT \sum_{k=1}^M \left\{ B_k \left[\rho_m N_0^{m-i} \right]^k \right\} \quad (1)$$

where ρ_m is the density at the lowest pressure, N_0 is the cell constant defined as the ratio of the total volume of main cell and expansion cell to the volume of main cell at zero pressure, B_k are the virial coefficients ($B_1 = 1$, B_2 is the second virial coefficient, B_3 is the third virial coefficient and etc.), R is the gas constant, and the subscripts i and m denote the value after the i -th and m -th (last) Burnett expansions, respectively. The parameters of the fit, ρ_m , N_0 and B_k , were obtained by minimizing the following objective function via a least-square routine based on the Levenberg-Marquardt algorithm:

$$F = \sum_{i=0}^N \left(p_i^{\text{cal}} - p_i^{\text{exp}} \right)^2 \quad (2)$$

where N is the number of experiment data points, and the superscripts “exp” and “cal” represent the experimental and calculated

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