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Thermodynamic properties of HFO-1243zf and their application in study on a refrigeration cycle

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HIGHLIGHTS

- All thermodynamic properties of 3,3,3-trifluoropropene (HFO-1243zf) are available.
- Accurate PC-SAFT equation of state for HFO-1243zf is firstly modeled.
- Uncertainties of vapor pressure and saturated liquid density are 0.15% and 0.80%.
- COP of cycle using HFO-1243zf is higher than that of cycle using R134a, R22, R32.

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ABSTRACT

Thermodynamic properties of HydroFluoro-Olefin, 3,3,3-trifluoropropene (HFO-1243zf) are firstly modeled with an accurate molecular based PC-SAFT equation of state (EOS). The average absolute deviations (AAD) between vapor pressures, saturated liquid densities from this developed PC-SAFT EOS and experimental data are 0.15% and 0.80%, respectively. The average absolute deviations between predicted gaseous pressures, sub-cooled liquid densities from the PC-SAFT EOS and experimental data are 0.91% and 0.92%, respectively. In this study, the developed PC-SAFT EOS for HFO-1243zf and other EOSs for R-134a, R22, and R32 are used in the investigation of a refrigeration cycle for air conditioning application. The results show that cycle using R1243zf as refrigerant has the highest coefficient of performance (COP) and it is a potential candidate for the replacement of R134a in a refrigeration cycle.

1. Introduction

Due to the global warming potential (GWP) and/or the ozone depletion potential (ODP) problems CFC and HCFC were phased out. Nowadays, some non-ozone depleting substances as perfluorocarbons (FCs), hydro-fluorocarbons (HFCs), and hydrocarbons (HCs) are being used as refrigerants. Many HCs are highly flammable and many FCs and HFCs have high GWP values thus the studies on potential alternative refrigerants have still been carried out in the world.

Some potential alternative candidates for the replacement of current refrigerants R134a, R22, R32 and so on are hydrofluoro-olefins (HFOs) because of their low GWP. In HFOs group, 2,3,3,3-tetrafluoropropene (HFO-1234yf) and trans-1,3,3,3-tetrafluoro propene (HFO-1234ze(E)) have recently been thoroughly investigated. Di Nicola et al. [1] carried out experimental study on vapor pressure. Tanaka and Higashi [2] measured all critical temperature (T_c), critical pressure (p_c), critical density (ρ_c), and vapor pressures. Tanaka et al. [3] and Higashi et al. [4] published their experimental data for vapor pressures, pvT properties, critical properties, and saturated densities of HFO-1234ze (E).

The above experimental data can not be used in the investigation of the energy performance of thermal cycles using the substances as refrigerants or working fluids because there are no data for entropy. The entropy can not be determined directly by experiment. In order to determine the entropy for full fluid region, equation of state must be used. Basing on the above experimental data, Lai et al. [5] developed a molecular based EOS for HFO-1234yf and Akasaka et al. [6] developed a multi-parameter EOS for HFO-1234yf. Akasaka [7] and Lai and Phan [8] also developed EOSs for HFO-1234ze (E). The thermodynamic properties of these potential alternative refrigerants were then used in the investigation of the energy performance of refrigeration cycles [9–11] and organic Rankine cycle [12].

Besides the two mentioned potential alternative refrigerants, HydroFluoro-Olefin, 3,3,3-trifluoropropene (HFO-1243zf) seems to

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be a potential one because it has a similar structure to that of HFO-1234yf which has a 100 year direct GWP of 4 and an ozone depletion potential (ODP) of zero [13]. The lower and upper flammability limits of HFO-1243zf are 3.83% and 15.0%, respectively [14]. Besides the flammability limits, the heat of combustion of HFO-1243zf is 14.3 MJ/kg [15]. Basing on the classification of the international organization for standardization, HFO-1243zf is classified as class 2.

Di Nicola et al. have recently published the Martin Hou EOS for HFO-1243zf but it is only valid for vapor phase [16]. Brown et al. [17] used group contribution method to predict critical properties, acentric factors, heat capacity and then used the Peng–Robinson equation of state to predict thermodynamic properties of eight fluorinated olefins including HFO-1243zf. The average absolute deviations between data from the Peng–Robinson cubic EOS and experimental liquid densities from Di Nicola et al. are 6.8% [16]. Due to the lack of other experimental data, the comparison for further data has not been carried out. Akasaka et al. [6] have recently pointed out that the Peng–Robinson cubic EOS from Brown et al. [17] is not very accurate. In details, deviations of vapor pressures of HFO-1234yf are always greater than 1% and reach 4% in the low temperature region. The Patel-Teja cubic EOS is more accurate than Peng–Robinson EOS in describing vapor pressures, Akasaka et al. [6]. Akasaka et al. [6] have also pointed out that the deviations of the predicted liquid density from the Patel-Teja EOS are mostly from 1% to 9%. The deviations of the predicted isobaric heat capacity from the Patel-Teja EOS are mostly from 12% to 35%.

Due to the well-known inaccuracy of the cubic EOS and the advantage of the molecular based EOS in extending to mixtures, following sections present our study on the thermodynamic properties of HFO-1243zf and the performance of refrigeration cycle using HFO-1243zf as refrigerant with an accurate molecular based equation of state.

2. Available data and ancillary equation

Brown et al. [18] have recently published 83 experimental vapor pressure data points for HFO-1243zf with temperature range of from 233.8 K to 372.68 K and vapor pressure from 0.053 MPa to 3.255 MPa. The uncertainties of temperature and pressure are ±0.003 K and of smaller than 1 kPa, respectively.

Critical temperature, critical pressure, and critical density together with sources for HFO-1243zf are given in Table 1. The relative differences of critical temperatures and critical pressures from Brown et al. [19] and those from Di Nicola et al. [16] are 0.055% and 2.969%, respectively. The difference between critical density from Brown et al. [19] and that from Di Nicola et al. [16] is 0.1%. The critical temperatures and critical pressures published by Brown et al. [18] and Di Nicola et al. [16] are identical. Brown et al. [18] have also published experimental vapor pressures used in this study and Di Nicola et al. [16] have also published experimental gaseous pressures, subcooled liquid densities, saturated liquid densities used in this study. Thus, the critical temperature, critical pressure, and critical density published in Di Nicola et al. [16] were used in this study.

Table 1
Critical temperature (T_c), critical pressure (p_c), critical density (ρ_c), and sources of the HFO-1243zf.

T_c (K)	p_c (MPa)	ρ_c (mol/l)	Source
378.59	3.6306	–	Brown et al. [18]
378.8	3.74	4.4039	Brown et al. [19]
378.59	3.6306	4.3995	Di Nicola et al. [16]

Di Nicola et al. [16] have recently measured pvT data of HFO-1243zf in both gaseous and liquid phases. In details, Di Nicola et al. [16] published 99 experimental data points for pressure in gaseous phase in the temperature range of from 278.15 K to 368.23 K and density in the range of from 0.107 mol/l to 0.336 mol/l. The standard uncertainties for temperature, pressure and density are 0.03 K, 1 kPa, and 0.05 kg/m, respectively. In sub-cooled liquid region, 302 experimental data points for liquid density were reported in the temperature range of from 283.15 K to 353.15 K and the pressure in range of from 1.297 MPa to 34.555 MPa. The standard uncertainties for temperature, pressure and density are 0.05 K, 1 kPa, and 0.8 kg/m^3, respectively. Temperature, pressure, and density ranges for all published experimental data are given in Table 2.

Basing on the measured sub-cooled liquid density and vapor pressure data, Di Nicola et al. [16] developed equation for saturated liquid density, Eq. (1).

$$\rho' = \rho_c\left(1+1.27983\tau^{1/3}+2.44894\tau^{2/3}-2.29514\tau+1.30957\tau^{4/3}\right) \quad (1)$$

Where $\tau = 1-T/T_c$. Table 3 presents saturated liquid densities generated from Eq. (1) for the development of equation of state for HFO-1243zf.

The above mentioned data can be used in the construction of a molecular based EOS to calculate pvT data in both single phase and two phase regions. In order to calculate caloric properties such as entropy, enthalpy of HFO-1243zf with the EOS, isobaric ideal gas heat capacity c_p^0 is required. The ideal gas isobaric heat capacity of HFO-1243zf has not been published thus Joback's method [20] is used in this study to calculate the ideal gas isobaric heat capacity as

$$c_p^0(\mathrm{J/mol\ K}) = D_0 + D_1\cdot T + D_2\cdot T^2 + D_3\cdot T^3, \quad (2)$$

where T is in Kelvin, $D_0 = -1.0861\mathrm{E}{+00}$, $D_1 = 5.1717\mathrm{E}{-02}$, $D_2 = -4.6100\mathrm{E}{-05}$, and $D_3 = -2.\ 0494\mathrm{E}{-08}$.

3. The PC-SAFT EOS for HFO-1243zf

The PC-SAFT EOS is the most popular molecular based EOS. The PC-SAFT EOS has recently been widely applied for various substances [21–23] and been used in the investigation of organic Rankine cycles [24,25]. The PC-SAFT EOS has been integrated into simulation software AspenOne. Thus, in this study, the PC-SAFT EOS for HFO-1243zf is developed for the calculation of thermodynamic properties and then is used to investigate refrigeration cycle using HFO-1243zf as refrigerant.

3.1. The PC-SAFT EOS

The PC-SAFT equation of state was developed by Gross and Sadowski [21] by modifying SAFT equation of state with an application of second-order perturbation theory of Barker and Henderson [26]. In perturbation theory, the interactions of molecules can be divided into a repulsive part and the attractive part. The repulsive contribution in the PC-SAFT EOS is calculated by using a

Table 2
Experimental pvT data for HFO-1243zf from Di Nicola et al. [16].

T_{min} (K)	T_{max} (K)	p_{min} (MPa)	p_{max} (MPa)	ρ_{min} (mol/l)	ρ_{max} (mol/l)	No. points	State
278.15	368.23	0.235	0.912	0.107	0.336	99	vapor
283.15	353.15	1.297	34.555	8.215	11.659	302	liquid