



ELSEVIER

Available online at www.sciencedirect.com

SciVerse ScienceDirect

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

Vapour–liquid equilibrium of binary systems containing pentafluorochemicals from 363 to 413 K: Measurement and modelling with Peng–Robinson and three SAFT-like equations of states

Elise El Ahmar^a, Alain Valtz^a, Patrice Paricaud^b, Christophe Coquelet^{a,d,*},
Laurent Abbas^c, Wissam Rached^c

^a MINES ParisTech, CEP/TEP – Centre Energétique et Procédés, 35 Rue Saint Honoré, 77305 Fontainebleau, France

^b Laboratoire de Chimie et Procédés, ENSTA-ParisTech, 32 Boulevard Victor, 75739 Paris Cedex 15, France

^c Thermodynamic, Refrigerant Applications, ARKEMA-CRRA BP63, Rue Henri Moissan, 69493 Pierre Bénite, France

^d Thermodynamics Research Unit, School of Chemical Engineering, University of KwaZulu-Natal, Howard College Campus, Durban, South Africa

ARTICLE INFO

Article history:

Received 8 March 2012

Received in revised form
23 May 2012

Accepted 25 May 2012

Available online 16 June 2012

Keywords:

Experimental data

Vapour

Liquid

Azeotropic refrigerant

HFC

Phase diagram

Critical point

Modelling

ABSTRACT

New sets of data are provided to characterize the phase equilibrium of new mixtures containing fluorochemicals and show their potential in energy recovery applications, as industrial heat pumps. Isothermal Vapour–Liquid Equilibrium data have been measured for R245fa + isopentane, and R365mfc + isopentane systems. Measurements were performed for four isotherms with pressure from 0.4 to 2.9 MPa. The data are correlated using different models (Peng–Robinson, PC-SAFT, polar PC-SAFT and SAFT-VR equations of state) and all four approaches can accurately describe the VLE. A very good description of the VLE for the pure components and the mixtures can be obtained by representing the R245fa and R365mfc molecules either as non-polar associating compounds or as non-associating dipolar molecules. To confirm the experimental values of the dipoles used in polar PC-SAFT, we performed DFT calculations of the permanent dipoles of the molecules and a good agreement with the experimental values is found for R245fa, while two different values corresponding to two different conformations were found for R365mfc.

© 2012 Elsevier Ltd and IIR. All rights reserved.

* Corresponding author. MINES ParisTech, CEP/TEP – Centre Energétique et Procédés, 35 Rue Saint Honoré, 77305 Fontainebleau, France. Tel.: +33 1 64694962; fax: +33 1 64694968.

E-mail address: Christophe.coquelet@mines-paristech.fr (C. Coquelet).

0140-7007/\$ – see front matter © 2012 Elsevier Ltd and IIR. All rights reserved.

<http://dx.doi.org/10.1016/j.ijrefrig.2012.05.016>

Données sur l'équilibre liquide-vapeur des systèmes binaires utilisant des substances pentafluorés entre 363 et 413 K : mesures et modélisation à l'aide d'équations d'état Peng-Robinson et trois équations d'état de type SAFT

Mots-clés : Données expérimentales ; Vapeur ; Liquide ; Frigorigène azeotropique ; HFC ; Diagramme de phase ; Point critique ; Modélisation

1. Introduction

Fluorochemicals have attracted great interest from industry because they possess remarkable properties which make them suitable for applications in a number of different areas. They are used as refrigerants, industrial heat pumps, fire extinguishing agents, dielectric media, solvents, and foam blowing agents, to name just a few applications. Thermodynamic properties are then required to design the production process of fluorochemicals or to develop models which can be used in heat pump/refrigeration, air conditioning etc.... The objective of this communication is to provide new sets of data to characterize phase equilibrium of two binary systems (R245fa + isopentane and R365mfc + isopentane). To the best of our knowledge, the only experimental data available in the literature corresponds to R245fa + isopentane system and it is reported by Lund et al. (1997). The particularity of these studied systems is the presence of an azeotrope. The new data have been described with the Peng–Robinson equation of state combined with the Huron–Vidal mixing rule (Huron and Vidal, 1979) and the NRTL activity coefficient model (Renon and Prausnitz, 1968) are chosen. The other models are three SAFT-like equations of state: SAFT-VR (Gil-Villegas et al., 1997; Galindo et al., 1998b), PC-SAFT (Nguyen Huynh et al., 2008a,b; Gross and Sadowski, 2001, 2002) and a polar version of PC-SAFT (Nguyen Huynh et al., 2008a,b). The authors want to highlight that the utilisation of SAFT-like equations are not easy and particularly at low temperatures were many pitfalls may appear. These pitfalls are well described in the papers of Polishuk (2011) and Privat et al. (2012, 2010).

This article is organized as follows. A presentation of the experimental setup used to investigate vapour–liquid equilibrium (VLE) of binary mixtures followed by the data treatment, results and discussion.

2. Experimental

2.1. Materials

R365mfc [$C_4H_5F_5$, CAS number: 406-58-6, 1.1.1.3.3 pentafluorobutane]; R245fa [$C_3H_3F_5$, CAS number: 460-73-1, 1.1.1.3.3 pentafluoropropane] and isopentane (later called iC5) [C_5H_{12} , CAS number: 78-78-4, 2-methylbutane] were supplied by Arkema with a certified volume purity greater than 98% (Table 1). Chemicals were used without any further purification, as GC

analysis of the chemicals did not indicate any significant impurities.

The apparatus that was used in the measurements is based on the “static-analytic” method and has been previously described by El Ahmar et al. (2011). Internal cell pressures are measured using two pressure transducers: (Druck, Type PTX 611, Range: (0–6) MPa) and (Druck, Type PTX 611, Range: (0–1) MPa). A dead weight pressure balance (Desgranges & Huot 5202S) is used for the pressure transducer calibration with the following uncertainties ± 0.2 kPa and ± 0.4 kPa for the low and high pressure range transducers, respectively. Temperature measurement was done via two platinum resistance thermometers probes (Pt-100 Ω) which are situated within each flange. The temperature probes were calibrated against a standard probe (25 Ω , TINSLEY) which was certified by the ‘Laboratoire National d’Essai’. Uncertainties in the temperature measurement are estimated to be within ± 0.04 K for both probes.

A gas chromatograph (Perichom, Model: PR-2100) equipped with a thermal conductivity detector (TCD) was used to analyse the equilibrium phase compositions. The column used in the gas chromatograph was supplied by Resteck, France (5% Krytox/Carboblack B 60/80 mesh). Calibration of the detector was done by repeated injection of known amounts of each pure component into the injector of the gas chromatograph using a syringe. The estimated errors in the equilibrium phase composition are less than 0.012 for both the vapour and liquid mole phase.

For each equilibrium condition, at least five samples of both the vapour and liquid phases are withdrawn using the ROLSI™ samplers (Mines Paristech, France) and analysed in order to check for repeatability of measurements.

3. Modelling

We have selected three different models to correlate the experimental data. A φ – φ approach considering bubble point pressure is considered. The first one is directly based on a cubic equation of state: the Peng–Robinson equation of State (PR EoS) (Peng and Robinson, 1976) incorporating the Mathias–Copeman alpha function (ElAhmar et al., 2011), with the Huron–Vidal mixing rule (Huron and Vidal, 1979) involving the NRTL activity coefficient model (Renon and Prausnitz, 1968) is selected. The PR-HV-NRTL model contains three binary interaction parameters (α , τ_{12} , τ_{21}) adjustable to

Download English Version:

<https://daneshyari.com/en/article/790311>

Download Persian Version:

<https://daneshyari.com/article/790311>

[Daneshyari.com](https://daneshyari.com)