

Drenched Virial Quantity of the Environmentally Friendly Refrigerant Fluids: R365mfc

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Abstract: This work presents the saturated second Virial coefficient of new environmentally friendly refrigerants 1,1-difluoroethane (R152a), 1,1,1,3,3-pentafluorobutane (R365mfc) and their mixture. The vapor phase behavior of the mixture was investigated using the Virial equation of state combined with group contribution method of modified UNIFAC. The work has enabled a highly accurate predicted saturated second Virial coefficient data as function of composition in a temperature range of $T=260\text{K}$ to $T=380\text{K}$. The Tsonopoulos second Virial coefficient model has been investigated and compared with experimental data of McLinden et al from National Institute of Standard and Technology (NIST). The results yielded a maximum deviation of 4.06%, in a temperature range of $T=298-300\text{K}$, whereas, for a temperature range of $T=323-325\text{K}$ a maximum deviation less than 2.59% was recognized for R365mfc. A negative deviation less than 12.3% was achieved for R152a.

Keywords- R152a, R365mfc, Virial coefficient, Unifac, Tsonopoulos, McLinden

I. INTRODUCTION

The last two decades have witnessed a significant increase of the harmful materials of Chlorofluorocarbons (CFCs) and Hydro-chlorofluorocarbons (HCFCs) based refrigerants in the atmosphere. These materials have been widely used as solvents, foam blowing agents, aerosols and especially as refrigerants due to their preeminent properties such as stability, non-toxicity, non-flammability and availability. However, these substances have a harmful effect on the earth's protective ozone layer. Since the declaration of the Montreal protocol in 1987 the use of these substances is consequently regulated [1]. Moreover the CFCs had been detected as substances contributing to global warming. Nowadays the world leading countries have legalized to stop the consumption of CFCs by replacing them with HFCs [3-5].

This paper supports more accurate data of the saturated second Virial coefficient, as a necessary parameter in molecular thermodynamics, including the pure fluids and mixtures of R152a and R365mfc. This parameter could enable better understand of the fluid phase behavior for this mixture. The R152a is a HFC type refrigerant. This fluid has zero ODP and a GWP value of 120. The boiling point temperature at a pressure of $p=1.013\text{ bar}$ is $T_b=-24.0^\circ\text{C}$, the molecular weight $M=66.1\text{ kg/kmol}$. R152a is a medium pressure refrigerant for the medium temperature refrigeration range [2]. The physical, thermodynamic and refrigeration characteristics are similar to those of the refrigerants R12 and R134a. Although R152a is a good refrigerant substitute for R12, it is not used in its pure form because of its flammability (flammability limits 3.7–21.8% by volume in air). For this reason, R152a is labeled as "highly flammable". The R365mfc is a HFC type refrigerant. This fluid has zero ODP and a GWP value of 782. The boiling point temperature at a pressure $p=1.013\text{ bar}$ is $T_b=+41.4^\circ\text{C}$, the molecular weight is at $M=148.07\text{ kg/kmol}$. R365mfc is a new fluid which is mainly used for the production of rigid polyurethane foams used in insulation purposes where a liquid foaming agent with a low thermal conductivity and a high vapor pressure at low temperatures are needed. Regarding to thermodynamic properties and safety requirements, R365mfc is employed as a main component in binary blends with 7 or 13 mass% with 1,1,1,2,3,3,3-Heptafluoropropane (R227ea) in the production of liquid foaming agents [2]. Besides the fact that this fluid has no negative impact on the ozone layer, further environmental benefits can be achieved using R365mfc, like in the production of polyurethane foams.

II. PREDICTIVE MODELS

Beside the previous equations; the Virial equation of state was also used to predict the density of the vapor phase. The main advantage of this equation is its rigorous theoretical background to describe the behavior of mixtures, as the Virial coefficients can be connected to the potential functions of the intermolecular forces and has been widely used in statistical thermodynamics. The main disadvantage of this equation is its validity only for gases with low or moderate densities. Most commonly used in the power series expansion in volume for the compressibility factor:

$$Z = \frac{PV}{RT} = 1 + \frac{B}{V} + \frac{C}{V^2} + \dots \quad (1)$$

The lack of the information of the third Virial coefficient leads to the situation that this equation is written in one parameter form; whereas hardly any data are available for the third coefficient [6].

$$Z = 1 + \frac{BP}{RT} \quad (2)$$

Smith et al [2] recommended the use of the two parameter Virial EOS up to pressures of 15 bar and the three parameter form up to 50 bar. The extension of the Virial EOS to mixtures is a rigorous process and is based on theoretical rather than empirical grounds. The interaction between the gases are incorporated in the two parameter Virial EOS as the mixture second Virial coefficient, which is related to the pure component and cross second Virial coefficient for a binary systems using the quadratic mixing rule [8] :

$$B_{\text{mix}} = \sum_{i=1}^2 \sum_{j=1}^2 y_i y_j B_{ij} \quad (3)$$

Many second Virial coefficients which have been determined from experimental data are collected by Dymond and Smith [9] and also stored in the data banks like DDB [1]. In this work the method of Tsonopoulos [10] was used, which delivered good results for the prediction of this coefficient. The acentric factor, critical temperature and pressure for mixture were predicted according to Kay's rule [5]. In this method the parameter B can be expressed as:

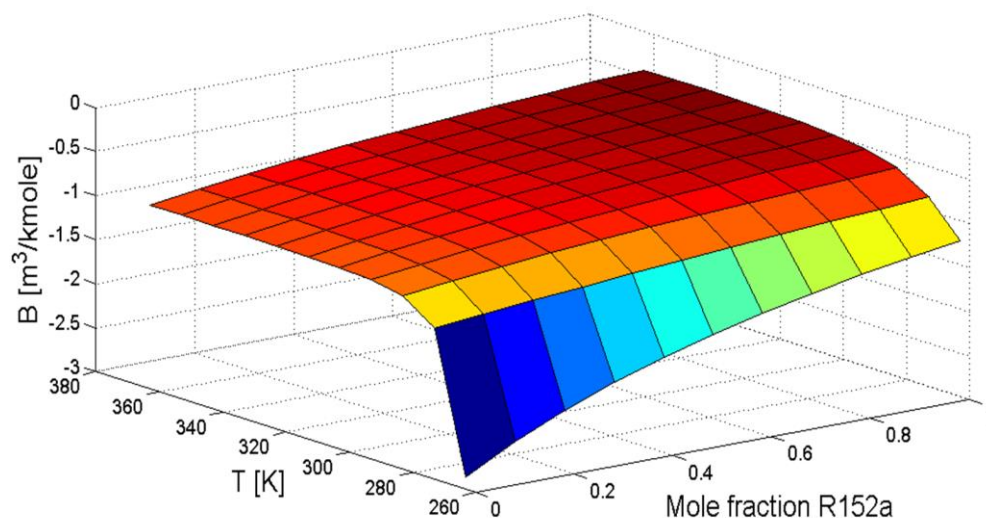


Fig.1. Temperature and composition dependent of the second virial coefficient of the system

III.RESULTS AND DISCUSSIONS

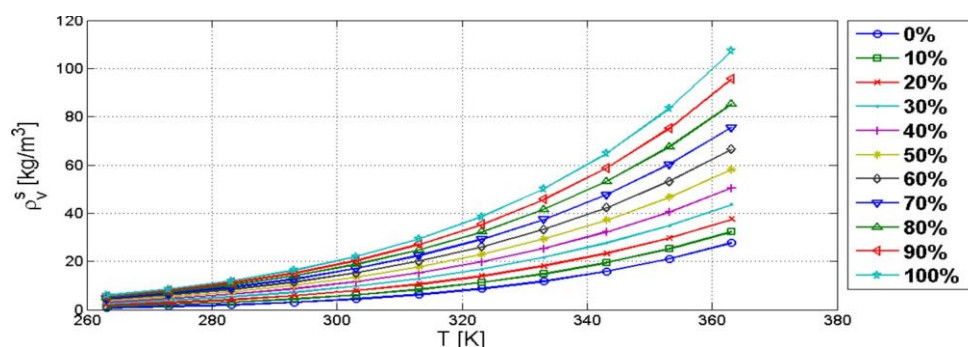


Fig.2. Saturated vapor density varying with temperature of the system R152a and R365mfc from modified UNIFAC-Virialequation.

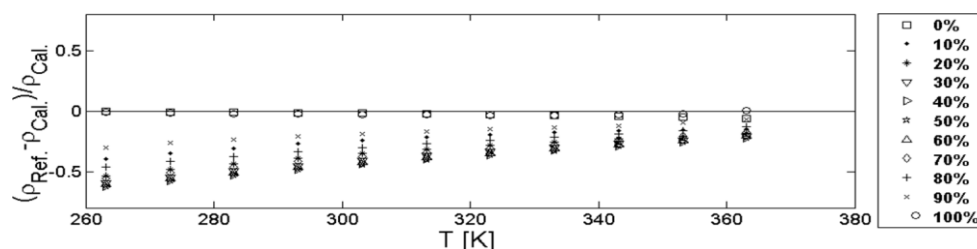


Fig.3. Relative deviation in saturated vapor density data for the system R152a and R365mfc from modified UNIFAC-Virial equation.

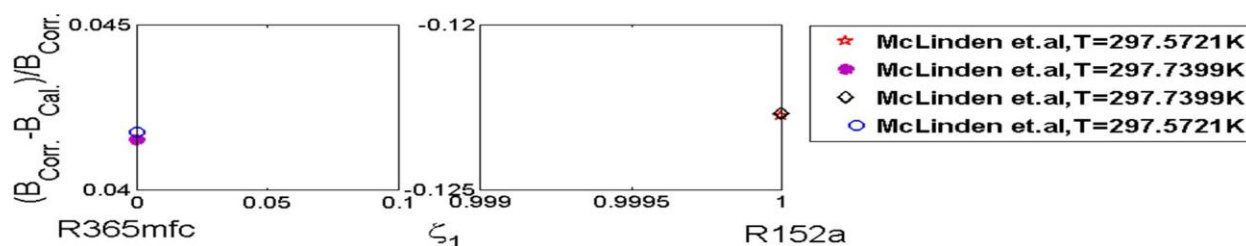


Fig.5. Relative deviation between our calculated and literature data of the second virial coefficient of R152a and R365mfc.

As is seen in Fig.1, the virial coefficients are composition and temperature dependent. The relation shows that the increase in

temperature will lead to increase the value of this parameter. At low temperature, the second virial coefficient is an always negative value, which indicates that the molar volume of the real gas is smaller than the corresponding molar volume of the ideal gas due to attractive interactions. Fig.2 illustrated the variation of vapor density with temperature predicted by virial equation. Fig.3. presented the relative deviation in saturated vapor density data for this system predicted by modified UNIFAC-Virial model, a maximum deviations reached on the way of increasing the composition of the high component R365mfc. Fig.4 explains the variation of the temperature and relative deviation to experimental data in second virial coefficient of pure R365mfc. As seen, the measurement was conducted in a saturation temperature range of $T=298-325\text{K}$ and pressure range of $p=0.58-1.44\text{bar}$. The data of McLinden et al. [15][16] has been investigated and compared with

Tsonopoulos [10] model. This model yielded a maximum deviation of 4.06%, in a temperature range of $T=298-300\text{K}$. Whereas, for a temperature range of $T=323-325\text{K}$ a maximum deviation less than 2.59% was recognized. Meanwhile, Fig.5 describes the same results executed for both pure fluids at temperature of $T=297.5721\text{K}$, 297.7399K , and a pressure of $p=4.76\text{bar}$, 4.19bar . The data of McLinden et al. [15] has reached a maximum deviation less than 4% in case of R365mfc, however a negative deviation less than 12.3% was achieved for R152a. Unfortunately, this model has failed to deliver satisfied results for mixture data.

IV.CONCLUSIONS

The work has delivered important thermodynamic data of the vapor density and second virial coefficient of the environmentally friendly system of R152a and R365mfc. The vapor phase behavior of the mixture was investigated using the Virial equation of state combined with group contribution method of modified UNIFAC. The Virial-Unifac model was chosen, since it is needed for providing reliable results for new refrigerants as well as a large range of applicability in the vapor phase. The second Virial coefficients by these models were compared with data obtained by the high precision fundamental equations of state by McLinden et.al from National Institute of Standard and Technology (NIST). The simulation results achieved good agreement with this model, particularly for the pure fluids.

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