

Isothermal (vapor + liquid) equilibrium measurements and correlation of the binary mixture 3,3,3-trifluoropropene (R1243zf) + isobutane (R600a) at temperatures from 283.15 to 323.15 K

Mesures d'équilibre isotherme (vapeur + liquide) et corrélation du mélange binaire 3,3,3- trifluoropropène (R1243zf) + isobutane (R600a) à des températures comprises entre 283,15 et 323,15 K

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ABSTRACT

The restrictions set by the F-gas Regulation and the Kigali Amendment to the Montreal Protocol have pushed an extensive research into alternatives for fluorinated greenhouse gases in air conditioning and refrigeration. Hydrofluoroolefins (HFOs) are emerging as promising substitutes for hydrofluorocarbons (HFCs) and hydrochlorofluorocarbons (HCFCs) in HVAC and refrigeration. Amongst these, R1243zf raised interests as low-GWP substitutes for R134a. The pursuit of low GWP refrigerants has also led to the examination of hydrocarbons (HCs), like propane (R290) and isobutane (R600a), due to their efficiency, low charge, and affordability, despite their flammability. The mixtures of R1243zf and isobutane could be of interest for medium temperature heat pump applications. Moreover, blending HFOs with HCs usually leads to azeotropic mixtures. While HCs benefit of a wide range of data and reliable Equations of State (EoS), HFOs, and in particular their mixtures, lack comprehensive information. This study reports vapor–liquid equilibrium (VLE) measurements for the 3,3,3-trifluoropropene (R1243zf) + isobutane (R600a) binary system in the temperature range between 283.15 K and 323.15 K. The measurements have been carried out by means of a vapor-recirculation apparatus combined with gas-chromatographic analysis. This work reports 53 experimental data with an expanded uncertainty ($k = 2$) of 0.003 mol mol⁻¹. The reported data, along with the data available in the literature, have been used to develop two new mixture models based on the Helmholtz free energy EoS, both leading to a significant improvement in the VLE prediction, with RMSE values lower than 0.005 mol mol⁻¹ for both the liquid and the vapor phase composition.

1. Introduction

In the recent decades, the refrigeration and heat pump industry has undergone significant transformation, driven by the research for environmentally friendly alternatives to conventional, environmentally harmful refrigerants. International regulations have been the main driver of this change. First, the introduction of the Kyoto Protocol (United Nations Environmental Programme, 1997) imposed

restrictions on ozone-depleting substances, such as the chlorofluorocarbons (CFCs), which represented the second generation of refrigerants. Subsequently, the Kigali Amendment to the Montreal Protocol (United Nations Environmental Programme, 2016) and the EU F-Gas Regulation (European Commission, 2014) introduced further limitations on refrigerant use, particularly targeting those with global warming potential (GWP) greater than 150. Hydrofluorocarbons (HFCs)

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became the most prominent refrigerants in the market, being efficient but associated with high GWP. R134a and R410A are the most widely used refrigerants, in particular for medium temperature applications, but they are characterized by GWP values of 1530 and 2256, respectively (IPCC, 2021).

In the pursuit for alternative refrigerants, several criteria are required for the fluids: low ODP and GWP, minimal flammability and toxicity, stability within refrigeration systems, compatibility with standard industry materials, and suitable thermophysical properties (Fedele et al., 2023b; McLinden et al., 2014). However, these alternatives must also deliver efficient performance in refrigeration cycles to avoid increasing indirect CO₂ emissions (Makhnatch and Khodabandeh, 2014). In response, potential substitutes for HFCs can be either natural (e.g., ammonia, CO₂, hydrocarbons) or synthetic refrigerants, with the choice often dictated by considerations of toxicity, flammability, and thermodynamic suitability for specific applications (Fedele et al., 2023b).

Numerous studies have examined the potential of hydrocarbons as refrigerants, specifically focusing on propane (R290), butane (R600), and isobutane (R600a), along with their combinations, as low-GWP alternatives to R134a and R410A (Nawaz et al., 2017; Rasti et al., 2012; Urchueguía et al., 2008). These hydrocarbons are of interest due to their favorable thermophysical properties and some research findings indicate that hydrocarbons may offer cycle efficiencies superior to those of HFCs. Furthermore, the adoption of hydrocarbons as refrigerants typically requires minimal adjustments to standard cycle configurations and materials. On the other hand, hydrocarbons are characterized by high flammability. Consequently, a considerable portion of research about this topic is focused on minimizing the refrigerant charge, as this parameter holds significant importance in terms of complying with safety regulations (Wu and Skye, 2018).

Concerning the synthetic refrigerants, McLinden et al. (2014) conducted an extensive screening on 1200 fluids against the aforementioned criteria, with the result that none fully met all the requirements. Thus, a trade-off is needed between safety and thermodynamic properties. Such research identified hydrofluoroolefins (HFOs), hydrochlorofluoroolefins (HCFOs), and hydrofluoroethers (HFEs) as potential alternatives. HFOs and HCFOs are hydrocarbons halogenated with chlorine or fluorine atoms characterized by at least one carbon–carbon double bond in their molecular structure, resulting in low GWP. However, these compounds also exhibit mild flammability and possible environmental compatibility issues. The decomposition of HFOs in the atmosphere can yield various compounds, such as trifluoroacetic acid (TFA), hydrogen fluoride (HF), carbonide fluoride (COF₂), and R23. However, only a few studies have been published so far about the environmental impact of such compounds, and it is still unclear whether this impact is negligible or not, also considering the quantities released in the environment (Fedele et al., 2023a). Moreover, the classification of HFOs and HCFOs as per- and polyfluoroalkyl substances (PFAS) is discussed within the European Commission, due to the inclusion of perfluorinated methyl (-CF₃) or perfluorinated methylene (-CF₂-) groups in their molecules. Anyway, a decision on the issue is still missing due to the controversial results of few studies which have been conducted on the topic, raising the need for further research (European Commission, 2023). Among HFOs, 3,3,3-trifluoropropene (R1243zf) is a flammable refrigerant (classified A2 by the ASHRAE Standard (ASHRAE, 2019)) characterized by low GWP and thermodynamic properties similar to R134a. Moreover, R1243zf is reported to be less expensive than R1234yf, which the most studied R134a alternative (Yao et al., 2020). Isobutane is well known for its good efficiency in refrigerating applications, thus the blend of isobutane and R1243zf might be as efficient as R134a but having a much lower GWP value. Moreover, Deng et al. (2020) highlighted the azeotropic behavior of the mixture R1243zf/isobutane for concentration of isobutane up to 20% by mass, which is usually an advantage in the design and installation processes of refrigerating devices.

Table 1

Details of the measured samples.

Substance	CAS Number	Supplier	Purity/mol.frac.
isobutane (R600a)	75-28-5	Sigma-Aldrich	0.9999
3,3,3-trifluoropropene (R1243zf)	677-21-4	Mexichem	0.9995

The lack of information about the thermophysical properties of HFOs has already been highlighted in the literature, especially concerning their mixtures (Bobbo et al., 2018; Fedele et al., 2023b). Concerning the mixture R1243zf/R600a, Deng et al. (2020) measured the vapor–liquid equilibria in the temperature range between 253.15 K and 293.15 K, while Tomassetti et al. (2019) measured the vapor density of the same mixture in the temperature range between 303 K and 383 K for four R600a mole fraction concentrations (0.225, 0.434, 0.898, 0.282).

The present work reports measurements of the vapor–liquid equilibria (VLE) of mixtures of R1243zf and isobutane carried out along five isotherms from 283.15 K to 323.15 K through a vapor-recirculating apparatus combined with a gas-chromatograph. The experimental data reported in this paper, along with the data available in the literature, have been employed to fit two novel mixture models for R1243zf/R600a systems based on the Helmholtz-energy-explicit formulation (Span, 2013).

2. Experimental section

2.1. Materials

Table 1 reports the details of the samples used within the experimental campaign. The samples underwent several cycles of freezing–pumping–thawing to reduce the quantity of incondensable gases; liquid nitrogen was employed for the freezing stage. The reported purities of the samples refer to the values measured with the gas-chromatographic analysis employing a thermal conductivity detector (TCD) after the degassing process.

2.2. Experimental apparatus

The experimental setup employed for this study has already been described in details by Bobbo et al. (1998), therefore only the most interesting details are reported in the following. The experimental setup (Fig. 1) consisted of a visual VLE cell made of AISI 306 stainless steel. A magnetic pump is connected with the cell to apply a vigorous recirculation of the vapor phase through the liquid phase. At the top and the bottom of the cell, two miniature valves enable the extraction of small quantities of liquid and vapor samples to send to the gas-chromatograph (GC). The VLE cell and the magnetic pump are immersed in a thermostatic bath filled with approximately 100 L of water. The temperature in such bath is controlled by the combination of a PID-controlled electric heater and an auxiliary thermostatic bath. Such setup allows a temperature stability within ± 1 mK in the main thermostatic bath. A Hewlett-Packard 3458 multimeter continuously records the temperature measured by a 100 Ω platinum resistance thermometer with an accuracy of ± 0.01 K. The pressure of the VLE cell is measured with a Ruska 6000 pressure gauge (full scale range of 17000 kPa and ± 0.8 kPa of accuracy). Between the pressure gauge and the measuring cell, a Ruska 2413 diaphragm is placed, which employs nitrogen as inert gas. Considering the stability of the system and the accuracy of the instruments, the combined standard uncertainties ($k = 1$) of temperature and pressure were assessed to be 0.02 K and 1 kPa. The composition in the liquid and vapor samples is measured by means of a Hewlett Packard 6890 gas-chromatograph, which is equipped with a thermal conductivity detector (TCD) and a Porapak-Q column (2 m long, 1/8" diameter). The GC has been previously calibrated for the binary mixture R1243zf/R600a by means of eight calibration bottles

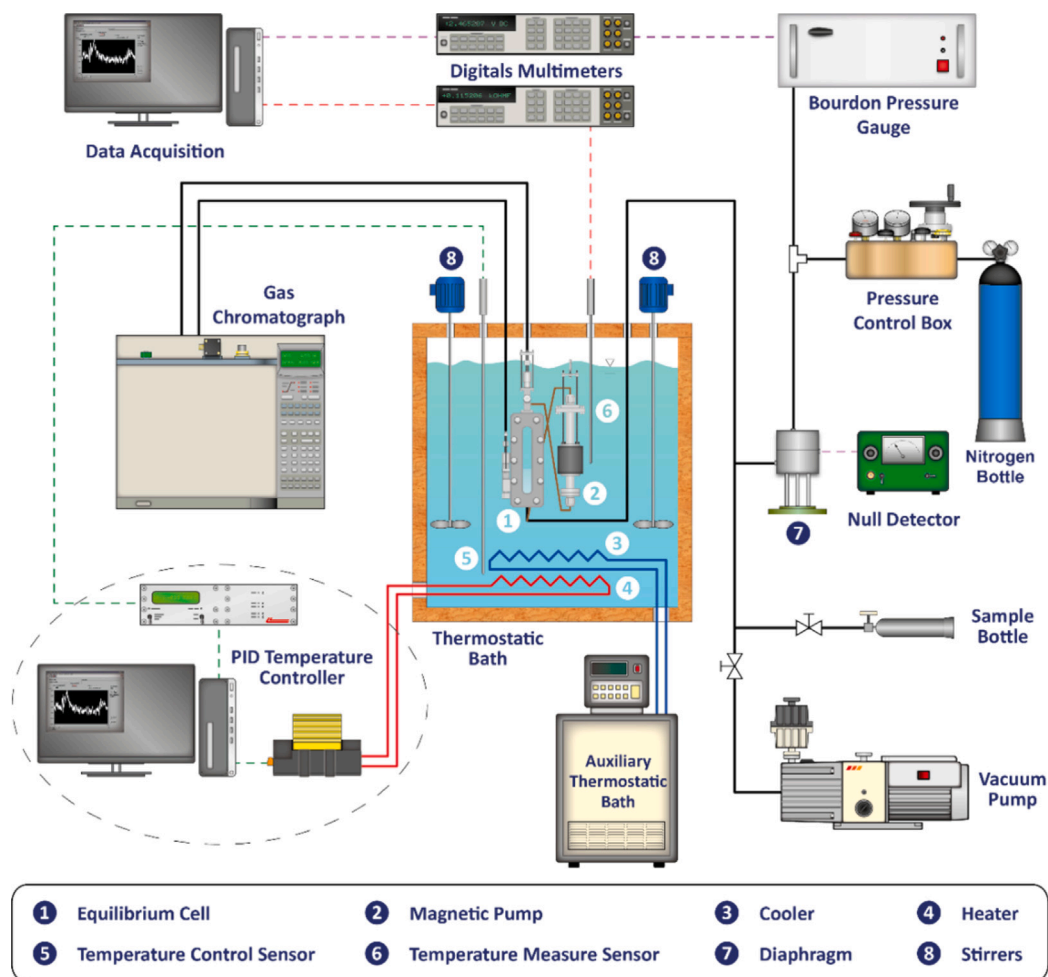


Fig. 1. Schematic of the VLE apparatus.

of known composition, which have been gravimetrically prepared. The expanded uncertainty ($k = 2$) in the mixture preparation is estimated equal to 0.3 mg, corresponding to an uncertainty of $0.0001 \text{ mol mol}^{-1}$ in terms of molar fraction (Bobbo et al., 1998). The calibration has been verified every day to check the stability of the system.

For each isotherm, first, the VLE cell was evacuated for at least three hours. Then, the low-pressure component (isobutane, in this case) was charged in order to have the sample in the two-phase with the liquid level reaching approximately half of the cell height. After this, a small amount of the high-pressure component (R1243zf, in this case) was charged. The content of the cell was mixed by recirculating an amount of vapor sample, extracted from the top of the cell, into the liquid sample at the bottom of the cell. To ensure that the equilibrium was reached inside the cell, such recirculation was carried out for 30 min. After the mixing, the cell was kept at rest for other 30 min. Finally, the equilibrium point was measured several times in a row until a deviation below $0.001 \text{ mol mol}^{-1}$ was obtained among the last three replicants (each replicant took approximately 5 min to be measured). Moving to the next equilibrium point in the same isotherm, another small amount of the high-pressure component was added to the cell and the same procedure was repeated. Once the isotherm was completed, the cell was evacuated and the procedure started from the beginning with another set-point temperature.

Considering the propagation of the aforementioned uncertainties in temperature, pressure and GC calibration and the reproducibility of the GC results, the expanded uncertainty ($k = 2$) in the liquid and vapor phase compositions is estimated to be within $0.003 \text{ mol mol}^{-1}$.

3. Results

The VLE behavior of mixtures of R1243zf and isobutane has been studied along five isotherms from 283.15 K to 323.15 K. The experimental data are reported in Table 2 and shown in Fig. 2, along with the literature data covering the same isotherms. In particular, an azeotropic behavior can be observed for the mixture for molar concentrations up to 20% of isobutane. The same behavior was observed by Deng et al. (2020).

4. Mixture model

The VLE data measured within this work have been used to fit two new mixture models for R1243zf/R600a systems, based on the Helmholtz-energy-explicit formulation (Span, 2013). In fitting the new model, all the other data available in literature have been included (Deng et al., 2020; Tomassetti et al., 2019). A detailed description of the model can be found in other sources (Span, 2013; Kunz and Wagner, 2012; Bell and Lemmon, 2016). Such model is implemented in the reference software Refprop 10.0 (Lemmon et al., 2018). For the pure fluids, an empirical formulation of the Helmholtz energy is needed as a function of the temperature and density. For mixtures, the model requires the explicit formulation of the Helmholtz energy for each pure component and mixing rules to calculate the thermodynamic properties of the mixture by differentiation. Often, the Helmholtz energy is given

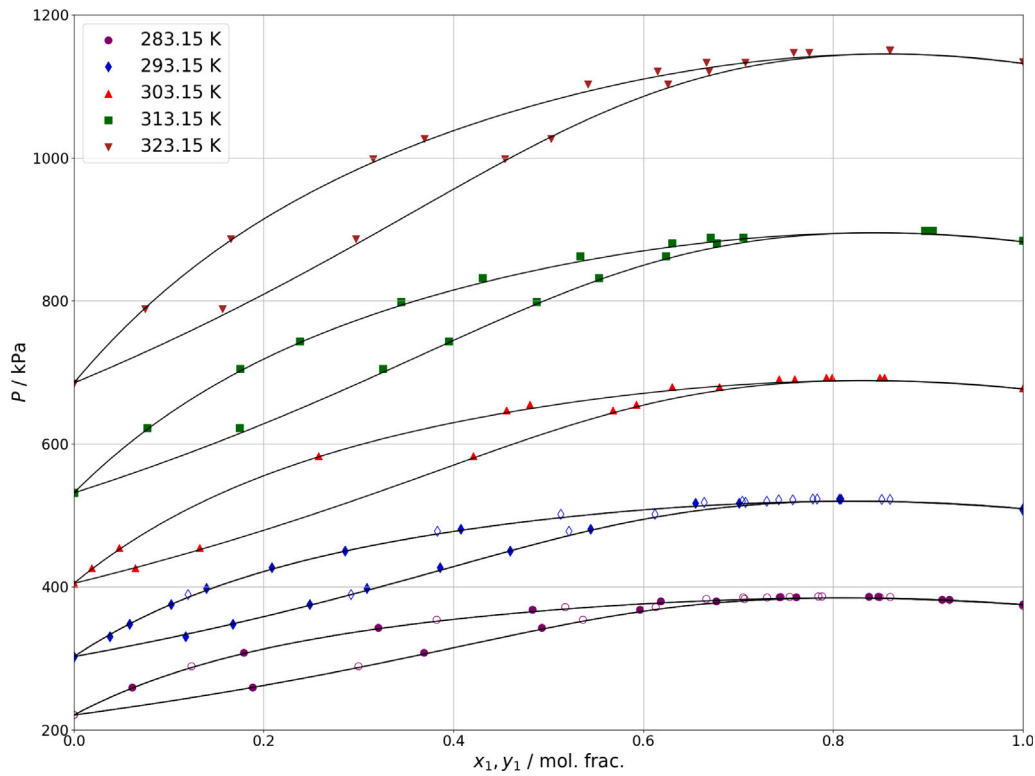


Fig. 2. VLE results for R1243zf/R600a systems. Full points: experimental data measured in this work; empty points: data measured by Deng et al. (2020); black solid line: model fitted in this work (M2, see Section 4).

as a function of the reduced temperature and density, τ and δ , as explained in Eq. (1). Eqs. (2)–(5) operate as mixing rule in the formulation of Kunz and Wagner (Kunz and Wagner, 2012).

$$\alpha(\tau, \delta) = \frac{a(T, \rho)}{RT} \quad (1)$$

with

$$\tau = \frac{T_r(\bar{x})}{T} \quad (2)$$

$$\delta = \frac{\rho}{\rho_r(\bar{x})} \quad (3)$$

$$\frac{1}{\rho_r(\bar{x})} = \sum_{i=1}^N x_i^2 \frac{1}{\rho_{c,i}} + \sum_{i=1}^{N-1} \sum_{j=i+1}^N 2x_i x_j \beta_{v,ij} \gamma_{v,ij} \frac{x_i + x_j}{\beta_{v,ij}^2 x_i + x_j} \cdot \frac{1}{8} \left(\frac{1}{\rho_{c,i}^{1/3}} + \frac{1}{\rho_{c,j}^{1/3}} \right)^3 \quad (4)$$

$$T_r(\bar{x}) = \sum_{i=1}^N x_i^2 T_{c,i} + \sum_{i=1}^{N-1} \sum_{j=i+1}^N 2x_i x_j \beta_{T,ij} \gamma_{T,ij} \frac{x_i + x_j}{\beta_{T,ij}^2 x_i + x_j} (T_{c,i} \cdot T_{c,j})^{0.5} \quad (5)$$

where α is the reduced Helmholtz energy; R is the universal gas constant; T and ρ represent temperature and density, respectively; $\bar{x}$ is the vector consisting of the molar concentration of each pure fluid in the mixture; the subscripts i and j refer to the i th and j th pure fluid consisting the mixture; the subscript c refers to the critical temperature or density; the subscript r refers to the reducing parameters. In Eqs. (4)–(5), the β_T , γ_T , β_v and γ_v are the four binary interaction parameters (BIPs), i.e. four tunable parameters to be fitted on experimental data for each binary mixture. In the absence of experimental data, Bell and Lemmon (Bell and Lemmon, 2016) proposed a correlation for calculating the BIPs based on the molecular weight of the single components consisting the mixture. In Refprop 10.0, the mixtures of R1243zf and isobutane employ BIPs calculated with such method, since no experimental data were available for the binary mixture when the software was released. Figs. 3–5 compare the experimental data available in the literature and the ones reported in this work with the liquid and vapor compositions and the density calculated with Refprop 10.0. An overall root mean square error (RMSE) of 0.0134 mol mol⁻¹ and 0.0124 mol mol⁻¹ was calculated for the VLE liquid and vapor compositions,

respectively, with respect to Refprop 10.0. While a RMSE of 0.55% was calculated for the density. It is worth to underline that, even though the BIPs are not fitted on experimental data, most of the density deviations were within the experimental uncertainty declared by Tomassetti et al. (2019).

In this work, two new mixture models have been developed by fitting the BIPs on the experimental VLE data presented here, along with all the other experimental data available in the literature. In particular, only the temperature-related BIPs, β_T and γ_T have been fitted, since the accuracy of Refprop 10.0 model in the density calculation was considered enough satisfying. The first mixture model (hereafter referred as M1) implemented the Equation of State (EoS) for R1243zf available in Refprop 10.0 and developed by Akasaka and Lemmon (Akasaka and Lemmon, 2019). The second model (hereafter referred as M2), instead, implemented an updated EoS developed by prof. Akasaka for R1243zf. Such EoS was obtained through private communication and included also vapor speed of sound data in the fitting, thus it was considered more reliable in the calculation of a wider set of thermodynamic properties. This equation will be published in the near future. In this work, the development of the mixture models was treated as an optimization problem, employing an Adaptive Search Development Particle Swarm Optimization (ASD-PSO) algorithm (Ardizzon et al., 2015). The optimized object function is shown in Eq. (6). Such function considered the absolute deviations between the model and the experimental vapor and liquid phase composition for the VLE and the relative deviations in the density calculation. In particular, the density deviations were calculated as the errors on the pressure given the experimental temperature and density as input, as described in Eq. (8), since it avoided iterative processes but it held the same accuracy (Bell, 2022).

$$f = \sqrt{\frac{1}{N} \sum_i res_{VLE,i}^2} + \sqrt{\frac{1}{N} \sum_i res_{PVT,i}^2} \quad (6)$$

$$res_{VLE} = \sqrt{(x_{model} - x_{exp})^2 + (y_{model} - y_{exp})^2} \quad (7)$$

Table 2

Experimental VLE data for R1243zf (1) + isobutane (2) in the temperature range between 283.15 K and 323.15 K. The combined standard uncertainties ($k = 1$) in the measured temperature and pressure are $U(T) = 0.02$ K and $U(p) = 1$ kPa. The expanded uncertainty ($k = 2$) in the molar fraction is $U(x_1) = 0.003$ mol mol⁻¹.

T/K	p/kPa	$x_1/\text{mol mol}^{-1}$	$y_1/\text{mol mol}^{-1}$
283.15	259.6	0.0615	0.1881
283.15	308.3	0.1792	0.3687
283.15	342.5	0.3207	0.4927
283.15	368.4	0.4830	0.5964
283.15	379.8	0.6180	0.6765
283.15	385.9	0.7435	0.7611
283.15	386.3	0.8475	0.8374
283.15	381.7	0.9225	0.9149
283.15	375.4	1.0000	1.0000
293.15	302.2	0.0000	0.0000
293.15	330.2	0.0379	0.1177
293.15	348.2	0.0584	0.1674
293.15	375.7	0.1024	0.2482
293.15	397.7	0.1397	0.3087
293.15	427.1	0.2087	0.3857
293.15	450.0	0.2859	0.4597
293.15	480.4	0.4074	0.5444
293.15	516.7	0.6551	0.7008
293.15	522.7	0.8064	0.8083
293.15	510.0	1.0000	1.0000
303.15	404.7	0.0000	0.0000
303.15	426.5	0.0188	0.0648
303.15	454.6	0.0475	0.1325
303.15	583.0	0.2577	0.4209
303.15	647.2	0.4556	0.5681
303.15	654.6	0.4805	0.5925
303.15	679.3	0.6302	0.6798
303.15	690.2	0.7432	0.7595
303.15	692.4	0.7928	0.7989
303.15	692.8	0.8538	0.8492
303.15	678.0	1.0000	1.0000
313.15	531.2	0.0000	0.0000
313.15	622.2	0.0773	0.1746
313.15	705.3	0.1750	0.3256
313.15	743.3	0.2383	0.3950
313.15	798.4	0.3446	0.4875
313.15	832.0	0.4308	0.5529
313.15	862.5	0.5332	0.6236
313.15	880.8	0.6300	0.6774
313.15	888.6	0.6707	0.7054
313.15	898.1	0.9049	0.8969
313.15	884.3	1.0000	1.0000
323.15	684.9	0.0000	0.0000
323.15	788.6	0.0748	0.1565
323.15	886.4	0.1652	0.2972
323.15	998.0	0.3153	0.4541
323.15	1026.5	0.3695	0.5027
323.15	1102.7	0.5416	0.6258
323.15	1120.6	0.6150	0.6689
323.15	1133.3	0.6664	0.7076
323.15	1147.2	0.7581	0.7749
323.15	1150.9	0.8598	0.8596
323.15	1134.0	1.0000	1.0000

Table 3

Comparison between the fitted parameters in M1 and M2 and the Refprop 10.0 default parameters for the R1243zf (1) + R600a (2) mixtures.

	Refprop 10.0	Fitted parameters (M1)	Fitted parameters (M2)
$\beta_{T,12}$	0.99275	0.99292	0.99268
$\gamma_{T,12}$	0.93536	0.94491	0.94491
$\beta_{v,12}$	1	1	1
$\gamma_{v,12}$	1	1	1

Table 4

RMSE comparison between Refprop 10.0 and the new models M1 and M2.

		Refprop 10.0	M1	M2
This work	RMSE(x)/mol.frac	0.0117	0.0048	0.0048
	RMSE(y)/mol.frac	0.0122	0.0044	0.0044
Deng et al. (2020)	RMSE(x)/mol.frac	0.0149	0.0046	0.0047
	RMSE(y)/mol.frac	0.0125	0.0038	0.0039
Tomassetti et al. (2019)	RMSE(ρ)/%	0.55	0.53	0.48

mol mol⁻¹ and 0.53% in the liquid phase composition, vapor phase composition and vapor density, respectively. For M2, the overall RMSE was equal to 0.0048 mol mol⁻¹ and 0.0042 mol mol⁻¹ for the liquid and vapor phase, respectively, and 0.48% for the vapor density. Figs. 3–4 show the VLE comparison in terms of liquid and vapor phase composition, respectively, between Refprop 10.0 and the models tuned in this work. As it can be noticed, the 92% of the experimental data resulted in absolute deviations lower than 0.01 mol mol⁻¹ with both M1 and M2. The same comparison is shown in Fig. 5 for the density. In this case, the default Refprop 10.0 model and M1 resulted in very similar deviations, while a slight reduction was observed in the density deviations for M2. The reason of this results can be found in the low sensitivity of the vapor density calculation to the binary interaction parameters β_T and γ_T . As aforementioned, only the temperature-dependent BIPs have been fitted because the Refprop 10.0 default parameters already resulted in an accurate prediction of the data presented by Tomassetti et al. (2019) and, by the way, also such data have been included in the fitting. It is worth to notice that the fitted BIPs and the results obtained for M1 and M2 are very similar, especially the VLE deviations. This can be explained considering that the R1243zf model used in M1 was already accurate, and the updated EoS employed in M2 was a refinement of the previous version with the purpose of including other newly available properties in the fitting.

5. Conclusion

In this work, the vapor–liquid equilibria of the binary mixture R1243zf+R600a has been measured along five isotherms at 283.15 K, 293.15 K, 303.15 K, 313.15 K and 323.15 K by means of a vapor-recirculation apparatus and the gas-chromatographic analysis. The experimental data measured in this work and the other literature data have been compared with mixture model available in Refprop 10.0, resulting in overall RMSE values of 0.0134 mol mol⁻¹ and 0.0124 mol mol⁻¹ in the liquid and vapor phase composition respectively, and 0.49% in the density. Then, two new mixture models have been developed by fitting two of binary interaction parameters (β_T and γ_T). One mixture model (referred as M1) employed the EoS for R1243zf already available in the Refprop 10.0 software, while the other mixture model (referred as M2) employed an updated EoS for R1243zf. The tuned model M1 resulted in RMSE values of 0.0047 mol mol⁻¹ and 0.0041 mol mol⁻¹ in the liquid and vapor phase composition respectively, and 0.53% in the density. Similar results have been obtained for the tuned model M2, which led to RMSE values of 0.0048 mol mol⁻¹ in the liquid phase composition, 0.0042 mol mol⁻¹ in the vapor phase composition and 0.48% in the density.

$$res_{PVT} = \frac{\rho_{model}(T, P, z) - \rho_{exp}}{\rho_{exp}} \approx \frac{\rho_{model}(T, P, z) - \rho_{exp}}{\rho_{exp}} \left(\frac{\partial \rho}{\partial p(T_{exp}, \rho_{exp})} \right) \quad (8)$$

Table 3 compares the BIPs employed in Refprop 10.0 for the mixtures of R1243zf and R600a with the BIPs fitted in this work considering the tuned model M1 and M2. Table 4 compares the RMSE values obtained with the new mixture models M1 and M2 with respect to Refprop 10.0 in terms of VLE vapor and liquid composition and density.

The new models led to a sensitive reduction in predicting the VLE, both in the liquid and the vapor phase, with respect to Refprop 10.0. For M1, the overall RMSE was equal to 0.0047 mol mol⁻¹, 0.0041

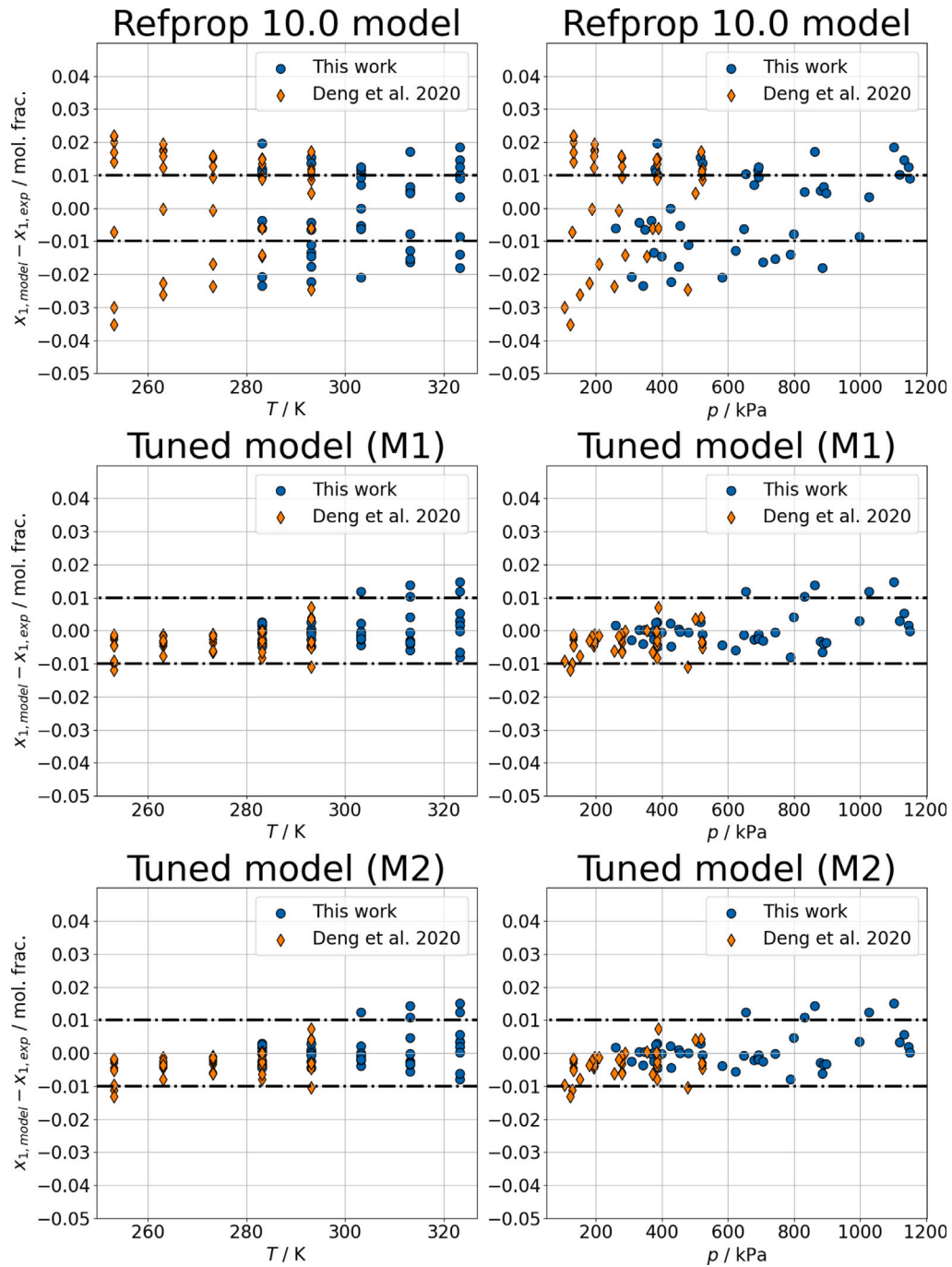


Fig. 3. Comparison between the Refprop 10.0 model and the mixture models tuned in this work (M1 and M2) in terms of deviation in the liquid phase composition with respect to temperature (left column) and pressure (right column).

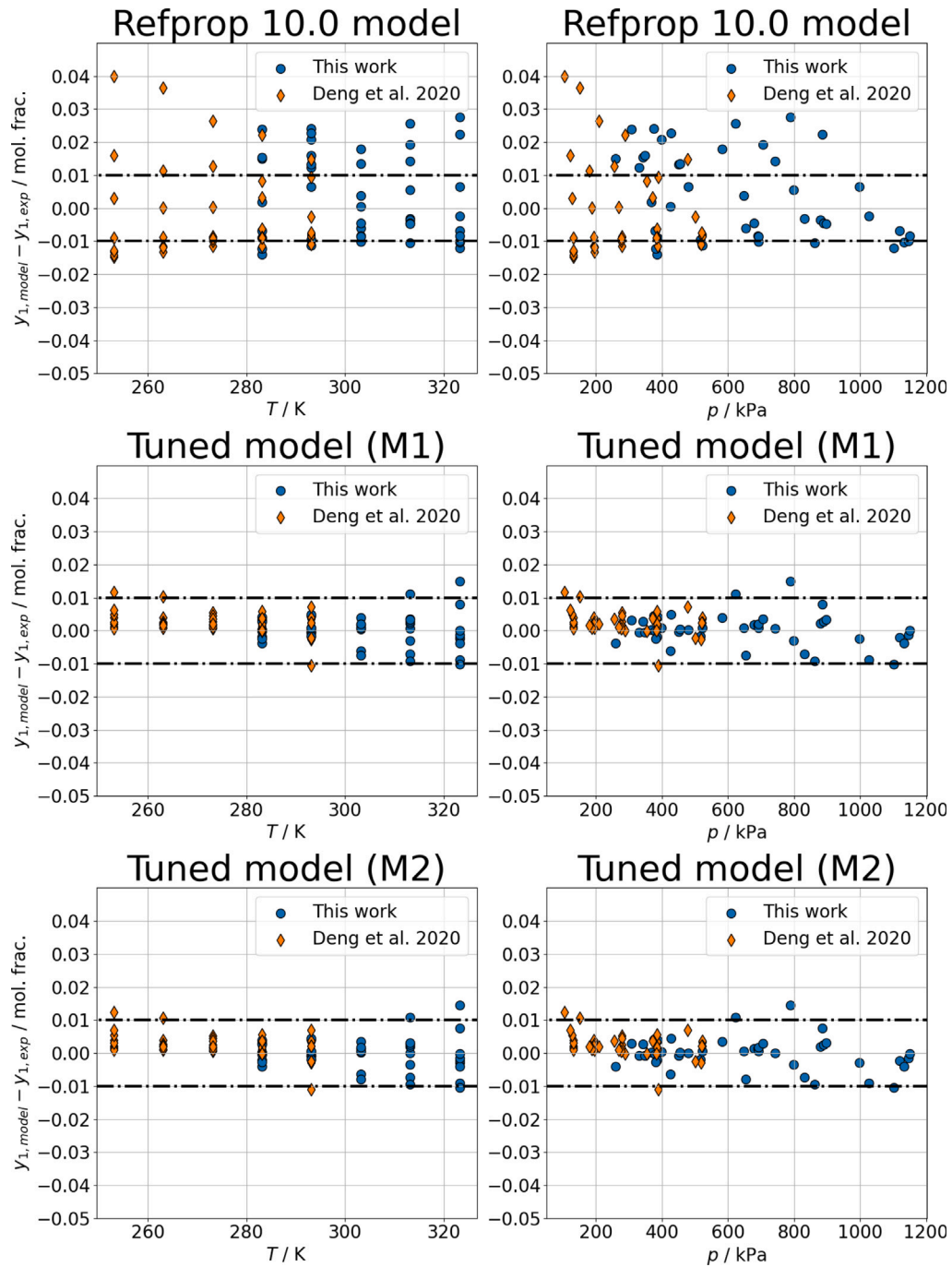


Fig. 4. Comparison between the Refprop 10.0 model and the mixture models tuned in this work (M1 and M2) in terms of deviation in the vapor phase composition with respect to temperature (left column) and pressure (right column).

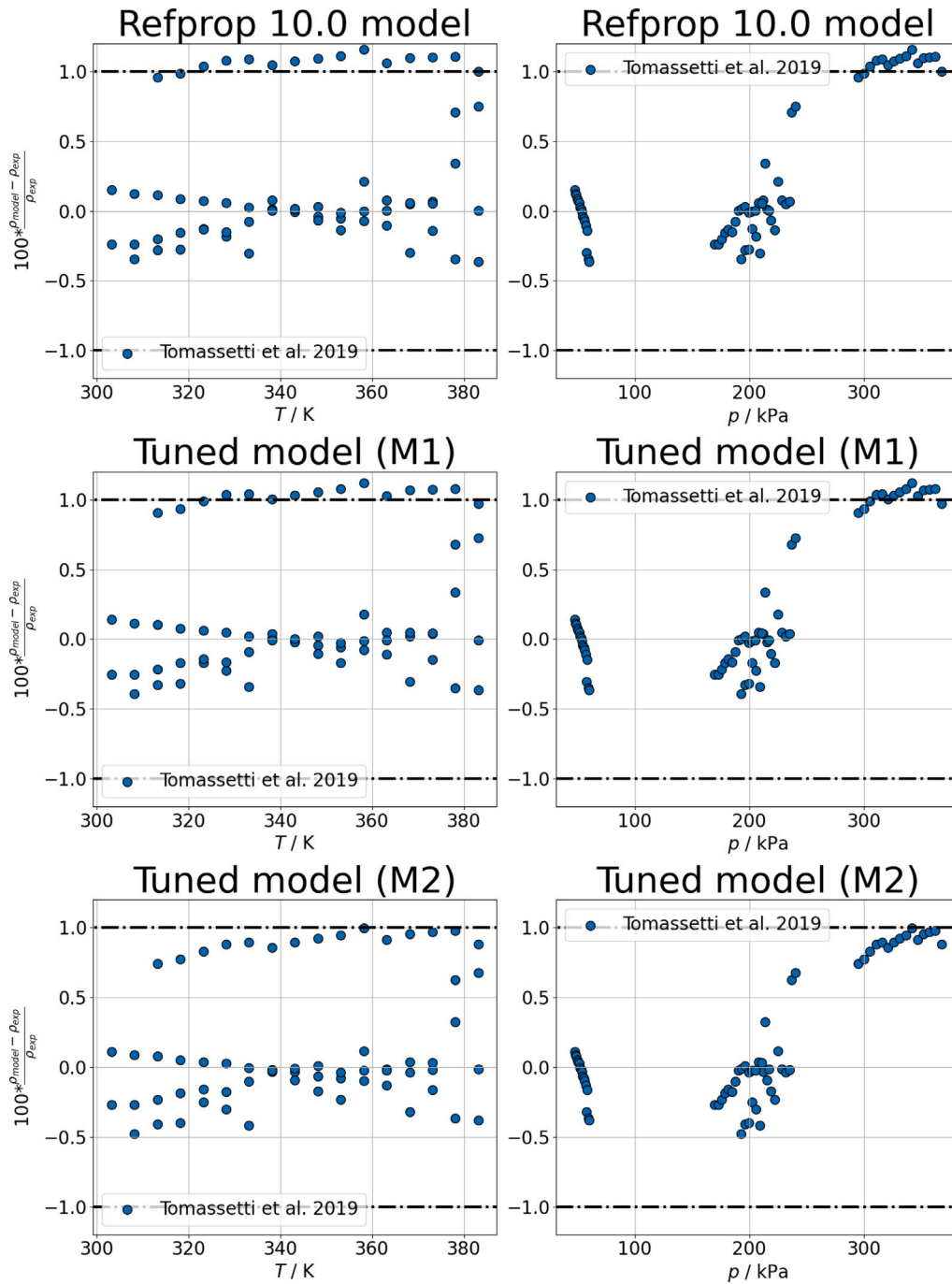


Fig. 5. Comparison between the Refprop 10.0 model and the mixture models tuned in this work (M1 and M2) in terms of density deviation with respect to temperature (left column) and pressure (right column).

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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