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## Thermophysical Property Model of Lubricant Oils and Their Mixtures with Refrigerants

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### ABSTRACT

In our previous work (Ind. Eng. Chem. Res. 2023, 62, 18736-18749), a modeling approach was developed to calculate all the essential thermophysical properties, including density, phase equilibria, heat capacity, entropy, enthalpy, viscosity, and thermal conductivity, of lubricant oils. This approach treats oil as a quasi-pure fluid, sets up a simple set of equations for the essential properties, and develops a parameter-fitting procedure using a minimal set of experimental data (fewer than 20 and at least 12 data points). This approach can be easily extended for mixture (e.g., oil + refrigerant) property prediction. Calculations using this approach generally agree with experimental data within the experimental uncertainty, except for up to 3% of quasi-pure oil density, 5% of the mixture's density, and several hundred percent of the mixture's viscosity. In this work, a new cubic equation of state (EoS) recently developed by us was adopted to replace the initially used Patel-Teja-Valderrama (PTV) EoS. As a result, for density, relative deviations were reduced to approximately 1.5% for quasi-pure oil and generally to 3.0% for mixtures. For viscosity, an improved residual entropy scaling (RES) approach was used, and a van der Waals-type mixing rule containing one adjustable parameter, which could be fitted to experimental data, was applied to the mixture's viscosity prediction. As a result, relative deviations for viscosity could be significantly reduced; however, they are still at the level of a few tens up to hundreds of percent. Careful evaluations of the mixture's viscosity data revealed that the uncertainty of the experimental data could be significantly higher than expected, and there is an apparent lack of high-quality viscosity data of oil + refrigerant mixtures. All fitted parameters of oils were implemented in OilMixProp 1.0, our self-developed software package, which was used for all calculations reported in this work (contact the authors; it is free for academic institutions).

### 1. INTRODUCTION

Every oil product available on the market usually comprises a base oil and various additives and impurities. They are essential in our daily lives, e.g., in cooking (olive oil, rapeseed oil, etc.) and health care (fish oil, etc.). Furthermore, they are indispensable in many technical applications, e.g., as lubricants in machinery such as compressors in refrigeration. Reliable knowledge of the thermophysical properties of oils and their mixtures with other fluids (e.g., refrigerants) is important to study the performance of refrigerators (chillers), heat pumps, and Rankine cycle machines. However, conventional modeling approaches such as multiparameter equations of state (EoS) cannot be used for oils, as these approaches are generally developed for pure fluids or mixtures with known constituents and composition.

In our previous work (Yang et al., 2023), we addressed the given challenge by developing a novel modeling approach to calculate all essential thermophysical properties of oils, including density, phase equilibria, heat capacity, entropy, enthalpy, viscosity, and thermal conductivity. This approach treats an oil as a quasi-pure fluid, establishes a simple set of equations for these essential properties, and develops a parameter fitting procedure using a minimal set of experimental data (less than 20 and at least 12 data points); it can be easily extended to mixtures

using simple mixing rules. The relative deviations of the calculations performed with this approach from the experimental data are generally within the experimental uncertainties. However, the deviation can be up to 3% for the density of a quasi-pure oil, 5% for the density of a mixture, and several hundred percent for mixture viscosity.

This work aims to improve the existing modeling approach focusing on density and viscosity. First, a comprehensive review of the experimental thermophysical properties of oils and mixtures of oil and refrigerant (or oil) was conducted (see Section 2). These data form the basis for improving the existing oil modeling approach. In addition, a new cubic equation of state (EoS) recently developed by us (Yang et al., 2024) was adopted to replace the initially used Patel-Teja-Valderrama (PTV) EoS (Patel & Teja, 1982; Valderrama, 1990), an improved residual entropy scaling (RES) approach for viscosity (Martinek et al., 2024; Yang & Richter, 2024a) was used, and a van der Waals (vdW)-type mixing rule with an adjustable parameter that could be fitted to experimental data was applied to the viscosity prediction of the mixture. These improvements are described in detail in Section 3 and were implemented in our self-developed software package OilMixProp 1.0 (contact the authors; it is free for academic institutions) (Yang & Richter, 2024b). This endeavor is funded within subproject 3 of the KETEC (Research Platform Refrigeration and Energy Technology) project (Urbanek et al., 2022).

## 2. DATA COLLECTION

A comprehensive collection of experimental data on the thermophysical properties of oils and oil + refrigerant mixtures (or oil) is underway. More than 7000 experimental data have been collected, and more are expected. The complete result will be submitted for publication in a peer-reviewed journal in the future. Due to the limited scope of this conference paper, only some density and viscosity data are presented, mainly related to the results section, as can be seen in Table 1 and Table 2.

**Table 1:** Experimental density data of quasi-pure oils, oil + oil mixtures, and oil + refrigerant mixtures

Oil or refrigerant	Oil	$T / K$	$P / MPa$	Points	Author and year
	POE5	270.0 – 470.0	0.5 – 50.1	164	(Bruno et al., 2019)
	POE7	270.0 – 470.0	0.5 – 50.0	161	(Bruno et al., 2019)
	POE9	290.0 – 470.0	0.5 – 50.1	145	(Bruno et al., 2019)
	ISO VG 32	248.2 – 348.2	0.1 – 0.1	5	(Morais et al., 2022)
	PEB8	263.8 – 412.9	0.1 – 0.1	5	(Fandiño et al., 2005)
	DIDP	273.8 – 413.3	0.1 – 140	55	(Peleties et al., 2010)
R744	DIDP	288.0 – 413.3	0.1 – 80	66	(Weerakajornsak, 2019)
PEB8	PEC7	278.2 – 353.2	0.1 – 45.0	99	(Fandiño et al., 2007)
R600a	LAB ISO 5	296.0 – 353.2	0.0 – 1.3	53	(Neto & Barbosa, 2010)
R744	POE5	303.2 – 353.2	10.0 – 60.0	113	(Pensado et al., 2008b)
R744	POE7	303.2 – 353.2	10.0 – 60.0	110	(Pensado et al., 2008b)
R744	POE9	303.2 – 353.2	15.0 – 60.0	93	(Pensado et al., 2008b)
R744	PEB8	303.2 – 353.2	10.0 – 60.0	110	(Pensado et al., 2008a)
R1234yf	ISO VG 32	248.2 – 348.2	0.0 – 0.6	33	(Morais et al., 2020)
R1234ze(E)	ISO VG 32	248.2 – 348.2	0.0 – 0.4	21	(Morais et al., 2020)
R134a	ISO VG 32	248.2 – 348.2	0.0 – 0.5	28	(Morais et al., 2022)
R125	ISO VG 32	248.2 – 348.2	0.0 – 0.6	27	(Morais et al., 2022)
R32	ISO VG 32	248.2 – 348.2	0.0 – 1.0	31	(Morais et al., 2022)

**Table 2:** Experimental viscosity data of quasi-pure oils, oil + oil mixtures, and oil + refrigerant mixtures

Oil or refrigerant	Oil	$T / K$	$P / MPa$	Points	Author and year
	POE5	275.1 – 430.1	0.1 – 137.4	269	(Bruno et al., 2019)
	POE7	280.0 – 450.1	0.1 – 137.5	286	(Bruno et al., 2019)
	POE9	289.9 – 450.1	0.0 – 137.7	161	(Bruno et al., 2019)
	ISO VG 32	248.2 – 348.2	0.1 – 0.1	5	(Morais et al., 2020)
	LAB ISO 5	281.0 – 353.0	0.0 – 0.0	9	(Neto & Barbosa, 2010)
	PEB8	303.2 – 363.0	0.1 – 0.1	14	(Pensado et al., 2006)
R744	DIDP	288.0 – 413.3	0.1 – 80	66	(Weerakajornsak, 2019)
PEB8	PEC7	303.2 – 353.2	0.1 – 60.0	84	(Lugo et al., 2007)

PEB8	PEC5	313.2 - 333.2	0.1 - 60.0	28	(Lugo et al., 2007)
R744	PEC5	303.2 - 353.2	10.0 - 60.0	113	(Pensado et al., 2008b)
R744	PEC7	303.2 - 353.2	10.0 - 60.0	110	(Pensado et al., 2008b)
R744	PEC9	303.2 - 353.2	15.0 - 60.0	93	(Pensado et al., 2008b)
R1234yf	ISO VG 32	248.2 - 348.2	0.0 - 0.6	33	(Morais et al., 2020)
R1234ze(E)	ISO VG 32	248.2 - 348.2	0.0 - 0.4	21	(Morais et al., 2020)
R134a	ISO VG 32	248.2 - 348.2	0.0 - 0.5	29	(Morais et al., 2020)
R125	ISO VG 32	248.2 - 348.2	0.0 - 0.6	27	(Morais et al., 2020)
R32	ISO VG 32	248.2 - 348.2	0.0 - 1.0	31	(Morais et al., 2020)

### 3. MODELS

Our previous work (Yang et al., 2023) describes the modeling approach for all essential thermophysical properties of oils and oil + other fluid mixtures. Only a brief overview is given here, and the new improvements are described in more detail.

#### 2.1 Overview

In our previous work (Yang et al., 2023), the PTV EoS was chosen to calculate density, phase equilibria, and residual properties. In this work, the recent EoS we developed (Yang et al., 2024) is used (see Section 2.2) instead. Heat capacities, entropy, and enthalpy can be determined with an additional equation for the isobaric heat capacity of the ideal gas as a linear function of temperature [linear- $c_p^o(T)$ ]. Viscosity and thermal conductivity can be calculated using the RES approach developed by Yang et al. (Yang, Kim, et al., 2021; Yang, Xiao, et al., 2021, 2022, 2023). Here, the latest improvement of the RES approach (Li et al., 2024; Martinek et al., 2024; Yang & Richter, 2024a) was adopted (see Section 2.3). Together, cubic EoS + linear  $c_p^o(T)$  + RES form the improved model set for calculating all essential thermophysical properties of a quasi-pure oil. For mixtures, the vdW mixing rule is used in the cubic EoS and a vdW-type mixing rule (see Section 2.3) was developed for the viscosity of mixtures.

#### 2.2 Cubic EoS

We recently developed a new cubic EoS (Yang et al., 2024) utilizing symbolic regression tools: TiSR (Martinek et al., 2023) and GPTIPS2F (available in <https://github.com/is-centre/gptips2f-matlab>). It has better accuracy in liquid density calculation than most other cubic EoS. The EoS has the functional form of a generalized three-parameter cubic EoS:

$$p = \frac{RT}{v - b} - \frac{a}{v^2 + (b + c)v - bc} \quad (1)$$

Here,  $p$ ,  $T$ , and  $v$  are pressure, temperature, and molar volume, respectively,  $R = 8.3144598 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  is the gas constant. Parameters  $a$ ,  $b$ , and  $c$  are:

$$a = \alpha \cdot \Omega_a \frac{R^2 T_c^2}{p_c} \quad (2)$$

$$b = \Omega_b \frac{RT_c}{p_c} \quad (3)$$

$$c = \Omega_c \frac{RT_c}{p_c} \quad (4)$$

where  $T_r = T/T_c$  is the reduced temperature, while  $T_c$ ,  $p_c$ , and  $\omega$  are the critical temperature, critical pressure, and acentric factor, respectively. The function  $\alpha$  and the parameters  $\Omega_a$ ,  $\Omega_b$ , and  $\Omega_c$  can be formulated to yield most of the existing cubic EoS (Yang, Rowland, et al., 2022). For the new EoS, they are:

$$\alpha = (1 + m \cdot (1 - T_r^{0.5}))^2 \quad (5)$$

$$m = n_{m,1} \cdot Z_c + n_{m,2} \cdot \omega Z_c + n_{m,3} \quad (6)$$

$$X = n_{X,1} \cdot \exp(-T_r^4) + n_{X,2} \cdot \exp(-T_r^3) + n_{X,3} \cdot Z_c + n_{X,4}, (X = \Omega_a, \Omega_b \text{ and } \xi_c) \quad (7)$$

$$\Omega_c = 1 - 3\xi_c \quad (8)$$

$$dX/dT = 0, (X = \Omega_a, \Omega_b \text{ and } \xi_c) \quad (9)$$

Here,  $\xi_c$  is an empirical critical compressibility factor different from the experimental one  $Z_c$ . In Eqs. (6) and (7), the forms were determined with symbolic regression tools, and the parameters, as listed in Table 3, were determined

with a nonlinear regression tool (the trust-region-reflective algorithm as implemented in the *lsqcurvefit* function in Matlab). For mixtures, the vdW mixing rule was used.

**Table 3:** Parameters of the new cubic EoS (Yang et al., 2024)

	$i = 1$	$i = 2$	$i = 3$	$i = 4$
$n_{m,i}$	2.779200	5.208803	-0.314477	
$n_{\Omega a,i}$	-0.174696	0.156625	-1.158565	0.784751
$n_{\Omega b,i}$	0.048371	-0.043334	0.319103	-0.012341
$n_{\zeta c,i}$	0.144894	-0.129835	0.957454	0.036884

### 2.3 Improved viscosity model

The viscosity of pure fluids is calculated as the sum of the dilute gas viscosity  $\mu_{p \rightarrow 0}$  and the residual part  $\mu^r$ :

$$\mu = \mu_{p \rightarrow 0} + \mu^r \quad (10)$$

The dilute gas viscosity  $\mu_{p \rightarrow 0}$  of a pure fluid and a mixture can be calculated with methods used in our previous work (Yang, Kim, et al., 2021; Yang, Xiao, et al., 2021, 2022, 2023). The residual part of viscosity  $\mu^r$  can be calculated with:

$$\mu^r = \frac{\mu^{r+} \rho_N^{2/3} \sqrt{mk_B T}}{(s^+)^{2/3}} \quad (11)$$

$$\ln(\mu^{r+} + 1) = n_{\mu 1} \cdot (s^+)^{1.8} + n_{\mu 2} \cdot (s^+)^{2.4} + n_{\mu 3} \cdot (s^+)^{2.8} \quad (12)$$

$$s^+ = -s^r/R \quad (13)$$

Here,  $\rho_N$ , in units of  $m^{-3}$ , is the number density,  $m$ , in units of kg, is the mass of one molecule,  $k_B = 1.380649 \cdot 10^{-23} \text{ J} \cdot \text{K}^{-1}$  is the Boltzmann constant, and  $s^r$  is the residual entropy. The number density  $\rho_N$  and residual entropy  $s^r$  of pure fluids and mixtures can be calculated with the cubic EoS. The three parameters  $n_{\mu k}$  ( $k = 1, 2, 3$ ) are fitted parameters for each pure or quasi-pure fluid. Eq. (12) is the latest developed equation optimized for the best possible viscosity calculation (Martinek et al., 2024). For mixtures, in Eq. (12), the  $n_{\mu k, \text{mix}}$  is utilized to substitute the parameters  $n_{\mu k, i}$  with a new vdW-type mixing rule developed in this work,

$$n_{k, \text{mix}} = \sum_i \sum_j x_i x_j n_{k, ij}, \quad n_{k, ij} = (1 - BIP_{\mu, ij}) \sqrt{n_{k, i} n_{k, j}}, \quad (k = 1, 2, 3) \quad (14)$$

where  $x_i$  is the mole fraction of component  $i$  in a mixture. The  $BIP_{\mu, ij}$  are binary interaction parameters for viscosity.  $BIP_{\mu, ij}$  can all be zero; when experimental data are available,  $BIP_{\mu, ij}$  ( $i \neq j$ ) can be optimized.

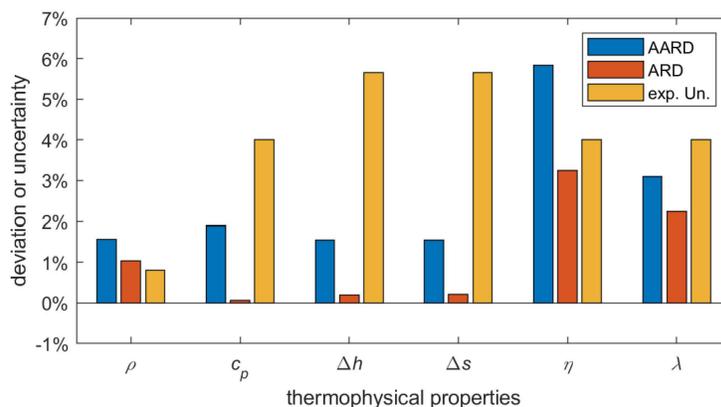
## 4. RESULTS

### 4.1 Feasibility study and performance tests

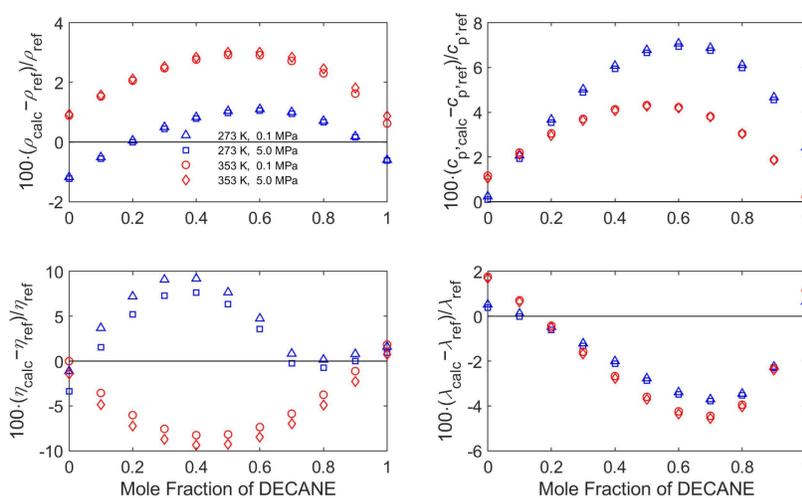
With the improved model set, the same feasibility study was carried out as in our previous work (Yang et al., 2023). In the following, the feasibility study is briefly described. According to the model set of cubic EoS + linear  $c_p^o(T)$  + RES, all parameters of a quasi-pure oil to be determined include: molar mass  $M$ , critical temperature  $T_c$ , critical density  $\rho_c$ , critical pressure  $p_c$ , acentric factor  $\omega$ , two parameters  $k_0, k_1$  in the linear- $c_p^o(T)$ , RES-fitted parameters for viscosity  $n_{\mu k}$  ( $k = 1, 2, 3$ ) and for thermal conductivity  $n_{\lambda k}$  ( $k = 1, 2, 3, 4$ ). These properties are characteristic constants of an oil. Most of the pure fluids in REFPROP 10.0 (Lemmon et al., 2018) that are in the liquid phase at atmospheric pressure  $p_{\text{atm}} = 0.1 \text{ MPa}$  and in the temperature range from  $T = (278.15 \text{ to } 368.15) \text{ K}$  were studied. The calculation results in this temperature and pressure range with REFPROP 10.0 are used as reference values to fit the characteristic constants of these pure fluids using the model set. With the fitted characteristic constants, the prediction capability of the model set was tested by calculating density  $\rho$ , isobaric heat capacity  $c_p$ , viscosity  $\mu$ , thermal conductivity  $\lambda$ , entropy increment  $\Delta s$ , and enthalpy increment  $\Delta h$  in enlarged temperature and pressure ranges (223.15 K to 473.15 K and up to 5.0 MPa) and comparing the results with values calculated with REFPROP 10.0. The results are summarized in Figure 1. In direct comparison to the previous work (Yang et al., 2023), the scattering of the density was reduced from 2.5% to 1.7% and that of the viscosity from 7% to 6%. Therefore, we can roughly estimate that, for pure fluids in the liquid phase, this modeling approach has an uncertainty ( $k = 2$ ) of less than 6% for viscosity, 3% for thermal conductivity, and 2% for all other properties.

The same binary systems Decane + C12 and Decane + MLINOLEA (here, fluid names as in REFPROP 10.0 are used) were studied to evaluate the prediction capability of the improved model set for mixtures. Both the previous and improved model sets work well for Decane + C12. In the previous work, calculations of Decane + MLINOLEA

were generally very good, except that deviations for viscosity were as high as 300%. In this work, with a value of  $BIP_{\mu,12} = 0.04$ , the deviation could be reduced to within 10 %, see Figure 2. This is a significant improvement as compared to the previous model set.



**Figure 1.** Average of the absolute value of relative deviation (AARD) and average relative deviation (ARD) between the improved model set and calculations of REFPROP 10.0 (Lemmon et al., 2018) for the studied pure fluids and typical experimental expanded uncertainty (exp. Un.). The calculations were carried out in the extended temperature (223.15 K to 473.15 K) and pressure (up to 5.0 MPa) ranges.

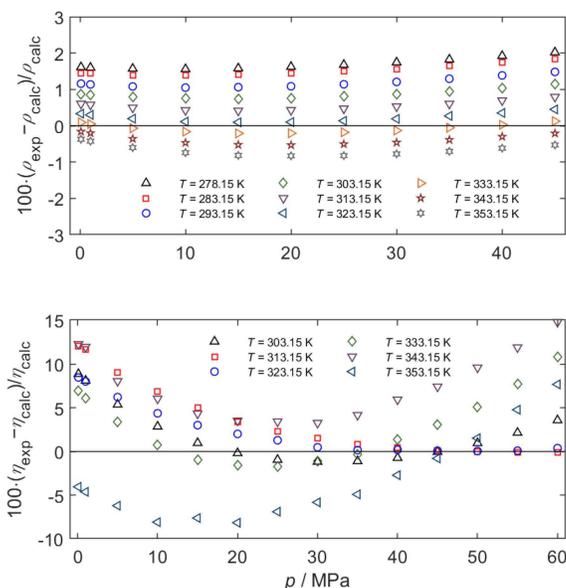


**Figure 2.** Relative deviations of calculations with the improved model set (subscripted with calc) from values calculated with REFPROP 10.0 (Lemmon et al., 2018) (subscripted with ref) for the binary system Decane + MLINOLEA. Here,  $BIP_{\mu,12} = 0.04$ .

## 4.2 Application to real oils

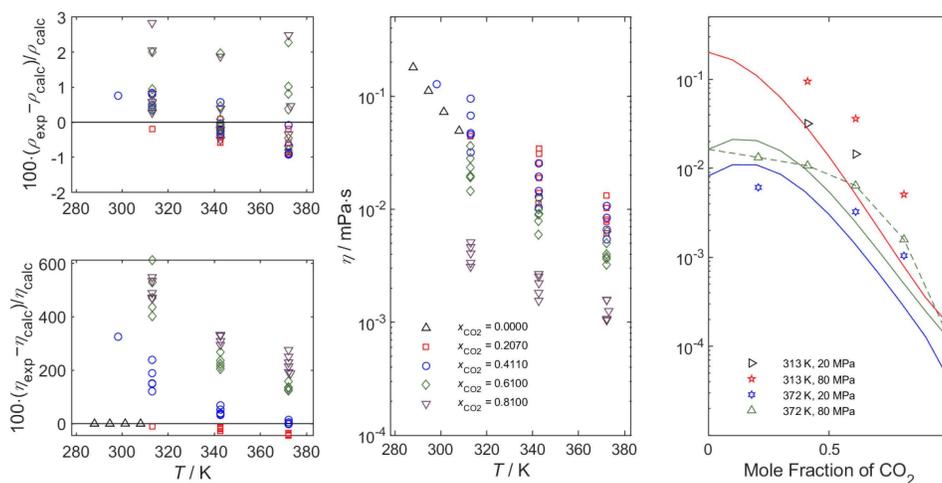
In this section, evaluations of the improved model set for real oil calculations are carried out. Due to the size limitation of this conference paper, only a few oils and their mixtures with other fluids are shown here. The studied experimental density and viscosity data are all listed in Table 1 and Table 2. The fitted characteristic constants of each oil and the binary interaction parameters  $BIP_{\mu,12}$  of each binary system have been implemented in OilMixProp 1.0 (contact the authors; it is free for academic institutions) (Yang & Richter, 2024b), and all the calculations were carried out with this software.

**4.2.1 PEB8 + POE7.** This binary system has been studied in previous works. PEB8 and POE7 (or PEC7 in some publications) are both lubricant oils having full names of pentaerythritol tetra(2-ethylhexanoate) and pentaerythritol tetraheptanoate, respectively. The relative deviations of the experimental literature data from calculations with the previous model set are generally within 3% for density and 30% for viscosity. In this work, with the improved model set, the relative deviations were reduced to 2% for density and 15 % for viscosity, as shown in Figure 3.



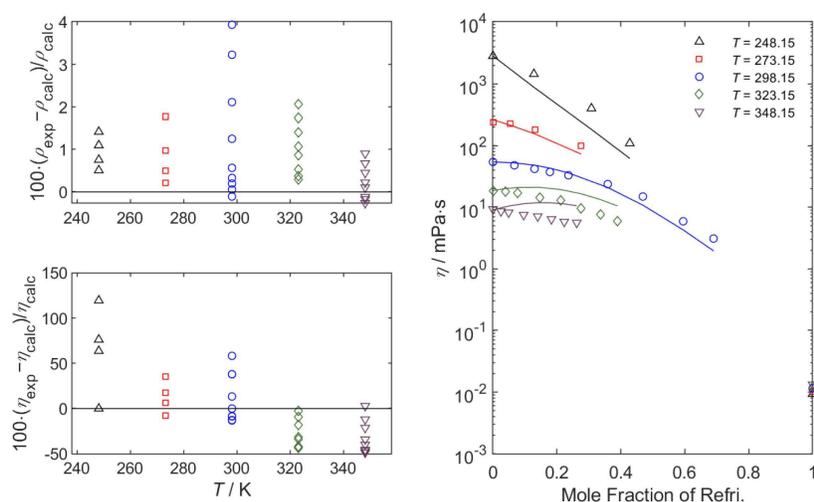
**Figure 3.** Relative deviations of experimental densities (Fandiño et al., 2007) and viscosities (Lugo et al., 2007) of PEB8 + POE7 from predictions of the model set. Here,  $BIP_{\mu,12} = 0.1$ .

**4.2.2 DIDP + CO<sub>2</sub>.** DIDP is a lubricant oil and is the abbreviation of di-isodecyl phthalate. In our previous work, the relative deviations of the experimental data of the DIDP + CO<sub>2</sub> binary system from the model predictions were within 5.5% for density and up to 450% for viscosity. In this work, the density deviation could be reduced to 3.0%, as shown in Figure 4. However, the viscosity prediction can hardly be improved for this binary system. Please see the viscosity vs. composition curves along constant temperature and pressure in Figure 4. The smooth solid curves are model predictions, and the unsmooth dashed curve (for clarity, only the one at  $T = 372$  K and  $p = 80$  MPa is plotted) is a connection of experimental points. The unsmooth dashed curve implies that there could be a large uncertainty in some of the experimental points, or it requires a much more complex mixing rule to yield a good correlation if all data were assumed to be accurate. By adjusting  $BIP_{\mu,12}$ , the relative deviation for viscosity could potentially be reduced to within 100%. However, the model prediction will then have an obvious positive slope in the viscosity vs. composition curves at oil-rich conditions (e.g., see the blue curve in Figure 4). This implies that adding CO<sub>2</sub> into DIDP will increase the viscosity at the same temperature and pressure condition, which is less likely to be true. On the one hand, the mixing rule for the mixture viscosity prediction needs further improvement. On the other hand, more accurate experimental data is needed for the improvement of the model.



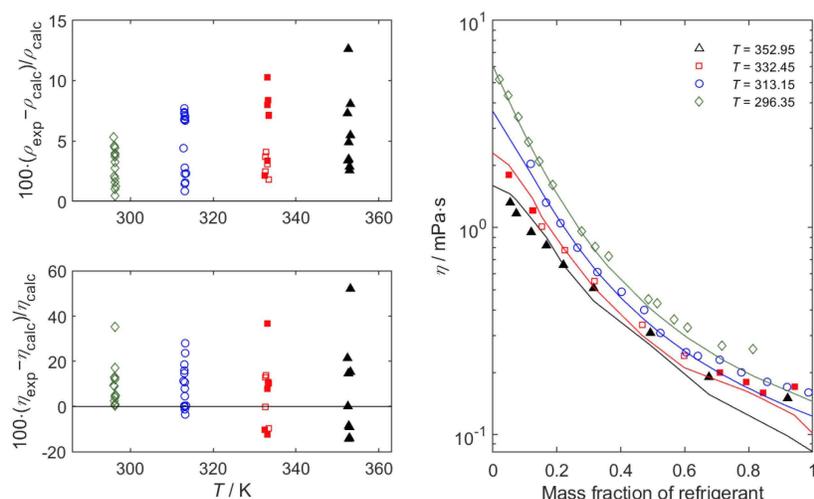
**Figure 4.** Relative deviations of experimental densities and viscosities (Weerakajornsak, 2019) of DIDP + CO<sub>2</sub> mixtures from predictions of the model set;  $x$  refers to mole fraction. Here,  $BIP_{\mu,12} = -0.15$ .

**4.2.3 ISO VG 32 + R1234yf.** As stated in the data source literature, the measured ISO VG 32 is Emkarate RL 32–3MAF obtained from the Lubrizol Corporation, USA. It is a lubricant oil mainly composed of pentaerythritol esters, such as *n*-heptanoate, *n*-pentanoate, 3,5,5-trimethylhexanoate, and 3-methylbutanoate. Data is available for ISO VG 32 mixed with five refrigerant gases. Here, only the mixture ISO VG 32 + R1234yf is shown as an example. The comparison between the experimental data and the model predictions is presented in Figure 5. The relative deviations of density and viscosity are generally less than 3.0% and 80%, respectively, except for a few outliers. Similar to the case of DIDP + CO<sub>2</sub>, an apparent positive slope in the viscosity vs. composition curves at oil-rich conditions (e.g., see brown curve in Figure 5) can be observed, which is most likely not true. A potential improvement could be making  $BIP_{\mu,12}$  a simple linear function of temperature, which should be further investigated.



**Figure 5.** Relative deviations of experimental densities and viscosities (Morais et al., 2020) of ISO VG 32 + R1234yf from predictions of the model set. Here,  $BIP_{\mu,12} = -0.6$ .

**4.2.4 LAB ISO 5 + isobutane.** LAB ISO 5 is a linear alkylbenzene lubricant oil. For its mixture with isobutane, the comparison between the experimental data and the model predictions is presented in Figure 6. Relative deviations of density are up to 10%. In this figure, data with full symbols are those considered to be in the two-phase region according to the model calculation. On the one hand, this may be attributed to the lack of bubble point pressure measurements necessary to determine an accurate BIP for the phase behavior calculation; on the other hand, it may imply that the experimental values have much higher uncertainties than expected.



**Figure 6.** Relative deviations of the experimental densities and viscosities (Neto & Barbosa, 2010) of LAB ISO 5 + isobutane from predictions of the model set. Here,  $BIP_{\mu,12} = -0.15$ . Data in full symbols are considered to be in the two-phase region according to the model calculation in OilMixProp 1.0.

## 5. CONCLUSIONS

A novel modeling approach was developed in our previous work to tackle the challenge of modeling all the essential thermophysical properties (density, phase behavior, heat capacity, entropy, enthalpy, viscosity, and thermal conductivity) of an oil. This approach was further improved in this work by implementing a new cubic EoS, an improved RES approach for viscosity, and a new mixing rule for mixture viscosity. In the liquid phase and not near the critical point, for pure fluids, this modeling approach has an estimated uncertainty of less than 6% for viscosity, 3% for thermal conductivity, and 2% for all other properties. For binary systems, the modeling approach still yields good predictions, typically within 4% for density and generally within 8% (according to the previous work) for other properties. However, a very high deviation is still observed for the viscosity of some binary mixtures. Careful evaluations of the mixture's viscosity data revealed that the uncertainty of the experimental data could be higher than expected, and there is an apparent lack of high-quality viscosity data of oil + refrigerant mixtures. A more complex mixing rule, for example,  $BIP_{\mu,12}$  as a linear function of temperature, could be used to improve the predictions of some binaries. All fitted parameters of oils were implemented in OilMixProp 1.0, our self-developed software package, which was used for all calculations reported in this work (contact the authors; it is free for academic institutions).

## NOMENCLATURE

$a$	parameter in the cubic EoS	(J·m <sup>3</sup> ·mol <sup>-2</sup> )
$b$ and $c$	parameter in the cubic EoS	(m <sup>3</sup> ·mol <sup>-1</sup> )
$BIP_{\mu}$	Binary interaction parameter for viscosity	(-)
$k_B$	Boltzmann constant	(J·K <sup>-1</sup> )
$m$	mass of one molecule	(kg)
$n_{uk}$ ( $k = 1,2,3$ )	viscosity parameters in RES	(-)
$p$	pressure	(Pa)
$R$	gas constant	(J·K <sup>-1</sup> ·mol <sup>-1</sup> )
$s^r$	residual entropy	(J·K <sup>-1</sup> ·mol <sup>-1</sup> )
$T$	temperature	(K)
$v$	molar volume	(m <sup>3</sup> ·mol <sup>-1</sup> )
$x$	Mole fraction	(-)
$Z_c$	Experimental critical compressibility factor	(-)
$\omega$	acentric factor	(-)
$\mu$	viscosity	(Pa·s)
$\mu^r$	residual viscosity	(Pa·s)
$\rho_N$	number density	(m <sup>-3</sup> )
$\Omega_a, \Omega_b$ and $\Omega_c$	parameter in the cubic EoS	(-)
$\xi_c$	empirical critical compressibility factor	(-)

### Subscript

c	critical point
$\rho \rightarrow 0$	dilute gas limit
r	reduced

## REFERENCES

- Bruno, T. J., Fortin, T. J., Huber, M. L., Laesecke, A., Lemmon, E. W., Mansfield, E., McLinden, M. O., Outcalt, S. L., Perkins, R. A., Urness, K. N., & Widgren, J. A. (2019). *Thermophysical properties of polyol ester lubricants* (NIST IR 8263; p. NIST IR 8263). National Institute of Standards and Technology. <https://doi.org/10.6028/NIST.IR.8263>
- Fandiño, O., Comuñas, M. J. P., Lugo, L., López, E. R., & Fernández, J. (2007). Density Measurements under Pressure for Mixtures of Pentaerythritol Ester Lubricants. Analysis of a Density–Viscosity Relationship. *Journal of Chemical & Engineering Data*, 52(4), 1429–1436. <https://doi.org/10.1021/jc700121n>
- Fandiño, O., Pensado, A. S., Lugo, L., Comuñas, M. J. P., & Fernández, J. (2005). Compressed Liquid Densities of Squalane and Pentaerythritol Tetra(2-ethylhexanoate). *Journal of Chemical & Engineering Data*, 50(3),

- 939–946. <https://doi.org/10.1021/je049580w>
- Lemmon, E. W., Bell, I. H., Huber, M. L., & McLinden, M. O. (2018). *NIST Standard Reference Database 23: Reference Fluid Thermodynamic and Transport Properties-REFPROP, Version 10.0, National Institute of Standards and Technology*. <https://doi.org/10.18434/T4/1502528>
- Li, Z., Yang, X., & Duan, Y. (2024). Linking Thermal Conductivity to Equations of State Using Residual Entropy Scaling Theory. *International Journal of Thermophysics*, (to be submitted).
- Lugo, L., Canet, X., Comuñas, M. J. P., Pensado, A. S., & Fernández, J. (2007). Dynamic Viscosity under Pressure for Mixtures of Pentaerythritol Ester Lubricants with 32 Viscosity Grade: Measurements and Modeling. *Industrial & Engineering Chemistry Research*, 46(6), 1826–1835. <https://doi.org/10.1021/ie061187r>
- Martinek, V., Frotscher, O., Richter, M., & Herzog, R. (2023). *Introducing Thermodynamics-Informed Symbolic Regression—A Tool for Thermodynamic Equations of State Development* (arXiv:2309.02805). arXiv. <https://doi.org/10.48550/arXiv.2309.02805>
- Martinek, V., Yang, X., Bell, I. H., Herzog, R., & Richter, M. (2024). Entropy scaling of viscosity IV - application to 124 industrially important fluids. *Journal of Chemical & Engineering Data*, (to be submitted).
- Morais, A. R. C., Simoni, L. D., Shiflett, M. B., & Scurto, A. M. (2020). Viscosity and Density of a Polyol Ester Lubricating Oil Saturated with Compressed Hydrofluoroolefin Refrigerants. *Journal of Chemical & Engineering Data*, 65(9), 4335–4346. <https://doi.org/10.1021/acs.jced.0c00431>
- Morais, A. R. C., Simoni, L. D., Shiflett, M. B., & Scurto, A. M. (2022). Viscosity and Density of an ISO VG 32 Polyol Ester Lubricant Saturated with Compressed Hydrofluorocarbon Gases: R-134a, R-32, and R-125. *Journal of Chemical & Engineering Data*, 67(8), 1824–1833. <https://doi.org/10.1021/acs.jced.2c00139>
- Neto, M. A. M., & Barbosa, J. R. (2010). Solubility, density and viscosity of mixtures of isobutane (R-600a) and a linear alkylbenzene lubricant oil. *Fluid Phase Equilibria*, 292(1), 7–12. <https://doi.org/10.1016/j.fluid.2009.12.029>
- Patel, N. C., & Teja, A. S. (1982). A new cubic equation of state for fluids and fluid mixtures. *Chemical Engineering Science*, 37(3), 463–473. [https://doi.org/10.1016/0009-2509\(82\)80099-7](https://doi.org/10.1016/0009-2509(82)80099-7)
- Peleties, F., Segovia, J. J., Trusler, J. P. M., & Vega-Maza, D. (2010). Thermodynamic properties and equation of state of liquid di-isodecyl phthalate at temperature between (273 and 423)K and at pressures up to 140MPa. *The Journal of Chemical Thermodynamics*, 42(5), 631–639. <https://doi.org/10.1016/j.jct.2009.12.002>
- Pensado, A. S., Comuñas, M. J. P., Lugo, L., & Fernández, J. (2006). High-Pressure Characterization of Dynamic Viscosity and Derived Properties for Squalane and Two Pentaerythritol Ester Lubricants: Pentaerythritol Tetra-2-ethylhexanoate and Pentaerythritol Tetrananoate. *Industrial & Engineering Chemistry Research*, 45(7), 2394–2404. <https://doi.org/10.1021/ie051275w>
- Pensado, A. S., Pádua, A. a. H., Comuñas, M. J. P., & Fernández, J. (2008a). High-pressure viscosity and density of carbon dioxide + pentaerythritol ester mixtures: Measurements and modeling. *AIChE Journal*, 54(6), 1625–1636. <https://doi.org/10.1002/aic.11473>
- Pensado, A. S., Pádua, A. A. H., Comuñas, M. J. P., & Fernández, J. (2008b). Viscosity and density measurements for carbon dioxide+pentaerythritol ester lubricant mixtures at low lubricant concentration. *The Journal of Supercritical Fluids*, 44(2), 172–185. <https://doi.org/10.1016/j.supflu.2007.10.004>
- Urbaneck, T., Matthes, M., Richter, M., Hempel, O., Safarik, M., Franzke, U., Noack, R., Honke, M., Müller, M., Henninger, S., Schossig, P., Henning, H.-M., de Oliveira, H. T., Morgenstern, A., Nienborg, B., Gschwander, S., Engelmann, P., & Benndorf, G. (2022, March 11). *Research Platform Refrigeration and Energy Technology (KETEC)*. [www.ketec.online](http://www.ketec.online)
- Valderrama, J. O. (1990). A Generalized Patel-Teja Equation of State for Polar and Nonpolar Fluids and Their Mixtures. *Journal of Chemical Engineering of Japan*, 23(1), 87–91. <https://doi.org/10.1252/jcej.23.87>
- Weerakajornsak, W. (2019). *Thermal conductivity of Polyol ester synthetic oil-CO2 mixtures*. Imperial College London.
- Yang, X., Hanzelmann, C., Feja, S., Trusler, J. M., & Richter, M. (2023). Thermophysical Property Modeling of Lubricant Oils and Their Mixtures with Refrigerants Using a Minimal Set of Experimental Data. *Industrial & Engineering Chemistry Research*, 62(44), 18736–18749.
- Yang, X., Kim, D., May, E. F., & Bell, I. H. (2021). Entropy Scaling of Thermal Conductivity: Application to Refrigerants and Their Mixtures. *Industrial & Engineering Chemistry Research*, 60(35), 13052–13070. <https://doi.org/10.1021/acs.iecr.1c02154>
- Yang, X., Ophelia Frotscher, & Richter, M. (2024). A new cubic equation of state developed with symbolic regression to improve liquid density calculation accuracy. *Industrial & Engineering Chemistry Research*, (to be submitted).
- Yang, X., & Richter, M. (2024a). Evaluation of cubic equations of state for viscosity and thermal conductivity

- calculation based on the residual entropy scaling approach. *International Journal of Thermodynamics*, (to be submitted).
- Yang, X., & Richter, M. (2024b). OilMixProp 1.0: Package for thermophysical properties of oils, common fluids and their mixtures. *Industrial & Engineering Chemistry Research*, (to be submitted).
- Yang, X., Rowland, D., Sampson, C. C., Falloon, P. E., & May, E. F. (2022). Evaluating cubic equations of state for predictions of solid-fluid equilibrium in liquefied natural gas production. *Fuel*, 314, 123033.
- Yang, X., Xiao, X., May, E. F., & Bell, I. H. (2021). Entropy Scaling of Viscosity—III: Application to Refrigerants and Their Mixtures. *Journal of Chemical & Engineering Data*, 66(3), 1385–1398. <https://doi.org/10.1021/acs.jced.0c01009>
- Yang, X., Xiao, X., Thol, M., Richter, M., & Bell, I. (2023). A Residual Entropy Scaling Approach for Viscosity of Refrigerants, other Fluids and their Mixtures. *NIST*. <https://www.nist.gov/publications/residual-entropy-scaling-approach-viscosity-refrigerants-other-fluids-and-their>
- Yang, X., Xiao, X., Thol, M., Richter, M., & Bell, I. H. (2022). Linking viscosity to equations of state using residual entropy scaling theory. *International Journal of Thermodynamics*, 43(12), 183.

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