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Effect of Refrigerant Properties Estimation on the Prediction Capabilities of Well-Established Two-Phase Heat Transfer and Pressure Drop Models for New Refrigerants

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Abstract. R1233zd(E) and R1224yd(Z) are two HCFO (Hydro Chloro Fluoro Olefin) low-GWP refrigerants recently proposed as substitutes of the HFC (Hydro Fluoro Carbon) fluids commonly used in air conditioning, high temperature heat pumps and ORC applications. A few experimental works regarding the two phase heat transfer in small diameter smooth and microfin tubes have already been published in the open literature. The estimations of thermophysical properties may have a remarkable impact on the prediction of the heat transfer coefficients and pressure drops, especially during two-phase heat transfer. The thermophysical properties databases and predictive tools for these refrigerants are continuously being updated and improved as additional, accurate measurements are published in the open literature. The present paper aims to highlight the impacts of thermophysical properties prediction models on the consistency of estimations of heat transfer coefficient and pressure drop using correlations published in the open literature. As a benchmark, some experimental heat transfer and pressure drop data collected for two new HCFOs, R1233zd(E) and R1224yd(Z) are used. The experimental database has been collected at the Department of Management and Engineering of the University of Padova. For the thermophysical properties estimations, different Equations of States contained in REFPROP as well as a more "simplified" approach based on group contribution methods coupled with a Peng-Robinson Equation of State, are considered.

1. Introduction

The ongoing international phase-down of traditional high GWP refrigerants is promoting a worldwide research activity for the investigation of new molecules as viable working fluids in vapour compression refrigeration and air conditioning systems, heat pumps and Organic Rankine Cycles. In order to assess the suitability of a new molecule as a working fluid, it is mandatory to properly evaluate its thermodynamic and thermophysical properties. The reliability of the prediction methods is strongly linked to the availability of experimental measurements of the relevant properties. Among the very preliminary information (for example from patents), molecular structure and normal boiling point

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(NBP) are usually available. Brown et al. [1] have shown that with this very limited data, one can use group contribution methods to provide preliminary though sufficiently good engineering estimations of the thermodynamic parameters necessary to construct a simple cubic equation of state, such as the Peng-Robinson EoS, which can then be used to provide a fair estimation of the refrigerant's performance potential in various applications. More thoroughly and complex modelling approaches are adopted in Refprop that is considered the reference database for refrigerants properties. Refprop is periodically updated and the reliability of the prediction models improves along with the availability of new experimental measurements of thermodynamic and thermophysical properties. In this paper reference is given to the last two releases of Refprop, i.e. 9.1 and 10.0 [2, 3]. Huber et al. [4] report the specific models adopted and the experimental data considered in Refprop v. 10.0.

In 2018, Bobbo et al. [5] published a review of available properties measurements for hydrofluorolefin (HFO) refrigerants. They concluded that, with the only exceptions of R1234yf and R1234ze(E), there is still a general need of experimental measurements of the main thermodynamic and, above all, thermophysical properties in order to develop reliable prediction methods. This is particularly evident for R1233zd(E).

On the basis on these conclusions, this paper mainly focuses on R1233zd(E); moreover, a new molecule R1224yd(Z) that has been only recently proposed and was not included in Bobbo et al. review [5], is also considered.

The estimation of thermodynamic and thermophysical properties have an impact on the experimental evaluation of heat transfer coefficients (HTC) and pressure drops (Δp). This consideration is highlighted in this work with reference to some recent measurements for flow boiling inside two micro-fin tubes [6, 7].

Furthermore, the models used for the estimation of these properties can modify the predictive potential of semiempirical models available in the literature for HTC and Δp estimations. Hence, in this paper several well-known HTC and Δp models are assessed while adopting the simplified group contribution with Peng Robinson EoS proposed in [1] or different releases of Refprop for the estimation of the thermodynamic and thermophysical properties.

2. The new HCFO fluids

In the following, the main features of the analysed equation of state (EoS) and of the approaches used for the estimation of the thermophysical properties are briefly described for R1233zd(E) and for R1224yd(Z). Some details about the reference database for flow boiling heat transfer of the studied fluids inside microfin tubes are reported too.

2.1. *R*1233zd(*E*)

The Peng Robinson EoS based on group contribution was implemented using critical parameters and normal boiling point of [8] that are the same used in Refprop 10.0.

Differently, the measurements of [9] were adopted for the first Refprop R1233zd(E).fld release dated back to 2013. Then, a step forward was made in 2015 by adding at a few new data on surface tension [10] collected at temperatures from 270 K to 360 K to the initially available three data points. Finally, a new R1233zd(E).fld release was proposed in 2017 (together with a new 10.0 Refprop.dll Version, [3]), where new EoS [8], new viscosity correlation was inserted, thanks to new measurements from X. Meng and from A. Miyara [4], and where new thermal conductivity measures by [11] were added.

Table 1 reports a comparison of the values of some relevant properties when using different versions. Regarding thermal conductivity, also the simple best fitting equation of Alam et al. [12] is reported.

In order to exploit the impact of properties modelling on heat transfer coefficient and pressure drops, the experimental measurements of [6] are considered. In that paper, the flow boiling of R1233zd(E) inside a microfin tube having inner diameter at fin tip of 4.2 mm, with 54 fins and a helix angle of 27° was considered at fixed saturation temperature (30 °C). Tests were run at different mass fluxes G= 100 \div 300 kg m⁻²s⁻², different heat flux (15 \div 90 kWm⁻²). Details about test section characteristics, test procedure and analysis are reported in [6].

1599 (2020) 012054 doi:10.1088/1742-6596/1599/1/012054

			1 1					
	Bias % = 100 (EoS value- Refprop 10 value) / Reprop 10 value							
Eos Type	Liq. c_P Vap. c_P Liq. Therm. cond		Vap. Therm. cond	Liq. Dyn. Visc.	Vap. Dyn. Visc.			
Refprop 9.1 (2015)	1.96	0.42	-6.48	-1.74	61.32	7.13		
Refprop 9.1 (2013)	0.00	0.00	-6.17	-1.75	61.71	7.18		
Peng- Robinson + Group Contribution	-1.89	-0.88	6.87	0.02	1.31	0.03		
Refprop 10 with thermal conductivity by Alam et al.	-	-	-1.61	-1.81	-	-		

Table 1. Deviation from Refprop	10.0 with different cald	culation approaches for	or some thermophysical
properties of R1233zd(E) at satura	ation pressure $p_{sat} = 1.54$	71 bar.	

2.2. *R1224yd*(*Z*)

The Peng Robinson EoS based on group contribution was implemented using critical parameters and normal boiling point according to [13], that where the first values available in the open literature.

R-1224yd(Z) was not available in Refprop 9. 1 and was firstly added to Refprop 10.0. It contains a Helmholtz energy EoS with 15 terms, according to [14]. According to [4], predictive-only methods for viscosity, thermal conductivity and surface tension were included since no experimental measurements are available.

Table 2 reports a comparison of the values of some relevant properties when using different versions. In order to exploit the impact of properties modelling on heat transfer coefficient and pressure drops, the experimental measurements of [7] are considered. The flow boiling of R1224yd(Z) inside a microfin tube having inner diameter at fin tip of 4.2 mm, with 40 fins and an helix angle of 18° was studied at fixed saturation temperature (30 °C) using the same test rig of [6]. Tests were run at different mass fluxes G= 100 ÷ 300 kg m⁻²s⁻² and different heat flux (15 ÷ 90 kWm⁻²). Details about test section characteristics, test procedure and data analysis are reported in [7].

1 I									
		Bias % = 100 (EoS value- Refprop 10 value) / Reprop 10 value							
				Vap. Therm.		Vap. Dyn.			
Eos Type	Liq. c _p	Vap. c _p	Liq. Therm. cond	cond	Liq. Dyn. Visc.	Visc.			
Peng- Robinson + Group Cont.	-5.83	-8.95	-6.75	8.18	8.34	9.49			

Table 2. Deviation from Refprop 10.0 with different calculation approach for some thermophysical properties of R1224yd(Z) at saturation pressure $p_{sat} = 1.7661$ bar.

3. Experimental assessment

In [6] and [7], the Newton's law of convection is used for the estimation of two-phase HTC, as it follows:

$$HTC = \frac{q}{A \left| t_{sat} - t_{wall} \right|} \tag{1}$$

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where the exchanged heat q, the reference surface area A and the wall temperature t_{wall} are measured values. The fluid saturation temperature (t_{sat}) is often estimated by means of the EoS, basing on the measured value of the saturation pressure. It is interesting to evaluate the uncertainty originated by the EoS prediction on t_{sat} estimation. This can be done assuming a set pressure measurement. Tables 3 and 4 compare the predictions of different EoS for R1233zd(E) and R1224yd(Z), respectively.

Table 3. Estimated saturation temperature values of R1233zd(E) for given saturation pressure $p_{sat} = 1.5471$ bar.

Eos Type	t_{sat} (°C)	ρι (kg m ⁻³)	$\rho_{v} (kg m^{-3})$	h1 (kJ kg ⁻¹)	h _v (kJ kg ⁻¹)
Refprop 10.0	30.000	1250.6	8.51	236.04	424.56
Refprop 9.1 (2015)	30.023	1250.6	8.50	237.14	426.16
Refprop 9.1 (2013)	29.999	1250.6	8.51	236.04	424.56
Peng-Robinson + GC	30.087	1283.3	8.43	234.96	424.41

Table 4. Estimated saturation temperature values of R1224yd(Z) for given saturation pressure $p_{sat} = 1.7661$ bar.

Eos Type	t _{sat} (°C)	ρι (kg m ⁻³)	$\rho_v (kg m^{-3})$	hı (kJ kg ⁻¹)	h _v (kJ kg ⁻¹)
Refprop 10.0	30.000	1347.2	11.172	233.52	395.02
Peng-Robinson + GC	29.643	1350.8	11.064	230.74	392.50

As a general comment, according to eq. (1) the lower the absolute difference between saturation and wall temperature the higher can be the uncertainty originated by the EoS estimations.

As a note, when using Peng Robinson EoS based on group contributions (GC), the uncertainty on saturation temperature for a given saturation pressure is similar to the uncertainty in the measurement of wall temperature (i.e. ± 0.1 K, as declared in [6] and [7]).

The EoS choice may have an impact also in the experimental determination of the frictional pressure drops component that is usually obtained from the measured total pressure drop (Δp_t) by subtracting the momentum pressure drop (Δp_a) and the inlet/outlet pressure drops (Δp_c) . When homogeneous model for the void fraction is used, Δp_a and Δp_c depend on the saturated liquid and vapour densities and on the vapour quality change along the test section. Any other void fraction model, except the mentioned homogeneous one, depends on one or more thermophysical properties. For example, the well-known Rouhani-Axelsson [15] model depends on the surface tension of the fluid. Hence, the model used for the prediction of the surface tension is a source of uncertainty in the frictional pressure drop determination. As an example, with reference to the pressure drops measurements in [6] and [7], the effect of the modelling approach for thermophysical properties on Δp_a and Δp_c is of a few Pa, that is one order of magnitude lower than the measurement uncertainty of pressure difference as declared by the authors of [6] and [7] (i.e. ±225 Pa).

3.1. Effect of thermodynamic and thermophysical properties estimation of predictive capabilities on heat transfer coefficient and pressure drops predictive models.

R1233zd(*E*) *heat transfer coefficient*. Righetti et al. [6] assessed their experimental HTC data with R1233zd(E) flow boiling inside a microfin tube against Padovan et al. [16], Diani et al. [17] and Rollmann and Spindler [18] models by using three different Refprop releases as mentioned above. By comparing their measurements with the similar results obtained with R134a (i.e. a very well known fluid, from the point of view of thermodynamic and thermophysical properties estimations) they observed that only the latest release of Refprop (i.e. the 10.0 one) was able to properly capture the HTC and Δp_f measurements. In this paper a fourth approach is used in order to exploit the potentiality

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of using simple best fitting equations in case that some experimental measurements of thermophysical properties are available. As a case study, the recent work of Alam et al. [12] is considered. Alam and co-authors presented a simple linear regression of saturated liquid and vapour R1233zd(E) thermal conductivity measurements from 303.52 to 413.16 K. They observed that the deviation of their measurements against Perkins et al. [11] ones was within $\pm 2\%$. So, the thermal conductivity estimations with these simple linear regressions, coupled with Refprop 10.0 database for all the other properties were used for the implementation of Padovan et al. [16], Diani et al. [17] and Rollmann and Spindler [18] models. Figure 1 reports the ratio of the heat transfer coefficients estimated with [16], [17] and [18] obtained using previous versions of Refprop (i.e. Refprop 9.1 with 2013 and 2015 fld file releases) or Refprop 10.0 with Alam et al. estimates for thermal conductivity against the reference value obtained with Refprop 10.0 alone.



Figure 1. Effects of the different modelling approach for the relevant properties on some heat transfer coefficients models during flow boiling in a microfin tube. R1233zd(E); data of [6].

It can be observed that the results with Alam et al. approach are pretty in line with the estimations obtained using Refprop 10.0 also for thermal conductivity and they are markedly better that the estimations obtained with Refprop 9.1 version using 2015 fld file release. It should be noted that this latter release did not include any thermal conductivity experimental value while Refprop 10.0 used [11] measurements to tune the same EcS approach adopted in 2015 release. These results highlight the fundamental relevance of properly tuning the thermal conductivity models against reliable experimental databases.

37th UIT Heat Transfer Conference

Journal of Physics: Conference Series

1599 (2020) 012054 doi:10.1088/1742-6596/1599/1/012054

R1224zd(Z) heat transfer coefficient. Figure 2 compares the values of the heat transfer coefficients estimated with [16], [17], [18] models using the simplified Peng Robinson EoS based on group contributions with reference to the measurements of [7]. Refprop 10.0 is taken as the baseline. Peng Robinson simplified approach always estimates heat transfer coefficients values that are around 10% lower than the estimates with Refprop 10.0.



Figure 2. Effects of the different modelling approach for the relevant properties on some heat transfer coefficients models during flow boiling in a microfin tube. R1224yd(Z); data of [7].

R1233zd(E) pressure drops. In [6], it was demonstrated that when using Refprop 10.0 with dynamic viscosity and surface tension prediction validated on experimental data, the Cavallini et al. [19] model was able to fairly capture the experimental frictional pressure drops obtained with the Rouhani and Axelsson [15] void fraction model for momentum pressure drops (MRE -2.7%; MAE 10%). In figure 3(a) it is evident that there is no appreciable difference between the predictions obtained with the 2013 and the 2015 versions of Refprop. Vice-versa, both "old" versions show a deviation of about ± 15 % in comparison with Refprop 10.0. This is a possible consequence of the lack of experimental validation of thermophysical properties (in particular the dynamic viscosity) in "old" Refprop versions.

R1224yd(Z) pressure drops. Figure 3(b) indicates that the Refprop 10.0 gives estimations that are very similar to the one obtained with the simplified group contributions method. It is worth to underline that no experimental data is available for the relevant thermophysical properties, so Refprop 10.0 is a predictive-only tool [4], like the simplified method here considered.



Figure 3. Effects of the different modelling approach for the relevant properties on some frictional pressure drops models during flow boiling in a microfin tube. (a): R1233zd(E), data of [6]. (b): R1224yd(Z), data of [7].

4. Conclusions

The estimation of saturation temperature with simple cubic equation of state based on group contribution methods for R1233zd(E) and R1224yd(Z) could lead to uncertainties in the order of 0.1 K when the saturation temperature is predicted from measured values of the saturation pressure. Accordingly, particular care should be given in the estimation of the total uncertainty of the experimental values of the heat transfer coefficient. Vice versa, the impact on frictional pressure drops appears only marginal.

On the basis of the experimental assessment based on heat transfer coefficients and frictional pressure drops obtained by some of the present authors during flow boiling of R1233zd(E) and R1224yd(Z) inside microfin tubes ([6], [7]), it emerges that the calibration of prediction models of thermal conductivity along the saturation boundaries is mandatory in order to increase the predictive capabilities of heat transfer coefficient models developed on databases not including the new fluids.

The dynamic viscosity and surface tension prediction models should be validated on experimental basis in order to obtain reliable frictional pressure drops predictions.

Therefore, further experimental activities are surely needed to improve the consistency of the experimental databases available for thermophysical properties.

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