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Surface tension of refrigerants: A new correlation using the boiling point as reference

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ABSTRACT

A new general corresponding-states correlation model for the calculation of the surface tension of refrigerants is proposed. The main difference with respect to other models available in the literature is that, in addition to the critical point temperature, the proposed model includes the temperature and surface tension values at the boiling point as input properties to define the reduced (non-dimensional) properties. Only three general adjustable coefficients are needed, which were obtained by a fitting procedure to the data presently available for 80 refrigerants. Averaged absolute deviations below 9.5% are found in all cases, being below 5% for 67 out of the 80 fluids considered. Results for another four correspondingstates models available in the literature are also obtained. The correlation model proposed here gives clearly better overall results, and it is the only one including exclusively temperature and surface tension values as inputs.

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1. Introduction

Surface tension plays an important role in the design of equipment involving gas-liquid contact in such processes as gas absorption, distillation, extraction, refrigeration, etc. [1,2]. Within the wide variety of fluids that can be considered, refrigerants are commonly used in both domestic and industrial processes. Particularly interesting are the so-called third and fourth generation refrigerants, which have zero ozone depletion and also low global warming potential, with RE347mcc being a clear example [3]. Fluids of this kind can be used as refrigerants, aerosol propellants, metered dose inhalers, blowing agents for polymer foam, heat transfer media, and gaseous dielectrics. An example of the importance of the surface tension of refrigerants is the fact that this property influences the nucleation of bubbles in evaporators and the drainage of condensation from condenser surfaces [4–6].

Many papers have been published about the performance and

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accuracy of the commonest empirical correlation models for the surface tension when used for various kinds of fluids [1,7–19]. The most frequently used correlations for thermodynamic properties along the saturation curve of fluids are based on the corresponding states principle [20], and they commonly include in the design of the model the critical point temperature as an input. Unfortunately, as some authors have noted [21–23], they do not always give good results far from this point, i.e., at low or intermediate temperatures. Apart from this, the models that use the corresponding states principle require the knowledge of at least 3 input properties, even with some of them not having any clear direct relationship with the surface tension (the acentric factor or the pressure at the critical point being clear examples).

To try to resolve these difficulties, we propose here a corresponding-states model in which the boiling point temperature and the surface tension at this point are taken as reference. As is well-known, the normal boiling point of fluids has been extensively studied, and in fact there are a great number of measurements of surface tension values at this point [24–29].

Focusing attention on refrigerants, one finds that the first extensive studies about the use of corresponding-states models for their surface tension are those carried out by Di Nicola et al. [12,15]. In 2011, those authors [12] proposed a new empirical relationship





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between the surface tension and temperature. The temperature, volume, and pressure at the critical point, the acentric factor, and the dipole moment were the input variables, and the proposed correlation contained seven coefficients determined in a fitting procedure. Results were obtained for 26 refrigerants, obtaining average absolute deviations below 5.1% except for R236ea. As indicated by the authors, when compared with previous general correlations, the improvement was greatest in the low temperature range.

In 2013, Di Nicola et al. [15] considered 29 refrigerants and proposed a new five-coefficient corresponding-states based correlation model. An important difference with respect to the previous one was that the critical volume and the dipole moment were excluded as inputs. The empirical correlation proposed is therefore simpler and gives better results than previous corresponding-states correlations, especially in the low temperature range. No comparison was made with their previous sevencoefficient model, but one can see in their results that these two equations had similar accuracies, with average absolute deviations greater than 2% for most of the fluids. The overall deviation for the 29 refrigerants was 3.20%, which was an improvement over previous models. In particular, the other model giving a similar result (3.99% of overall deviation) was that proposed by Migueu et al. [7], which used as inputs only the critical point temperature and volume, and the acentric factor.

Another recent general correlation model for the surface tension of fluids is that proposed by Gharagheizi et al. [11]. A gene expression programming strategy is applied to present two corresponding-states models to represent/predict the surface tension of about 1700 compounds (mostly organic) from 75 chemical families at various temperatures drawn from the DIPPR database. The most accurate model includes the critical point temperature, volume, and pressure, and the normal boiling point temperature as inputs. The overall deviation obtained is 18%, this high value being due to the large number of values included in the calculations. No specific results for refrigerants were given in the paper.

More recently, Cachadiña et al. [29] have proposed specific correlations for the surface tension of 83 refrigerants. They contain from 2 to 6 adjustable coefficients for each fluid, and are valid exclusively for the temperature range for which data are available. This kind of correlation is accurate, but a general model cannot be defined from it and neither can it be used for predictions outside the temperature range in which it holds nor, obviously, for other similar fluids.

In sum, there is currently no adequate general correspondingstates method that allows the surface tension of a large number of refrigerants to be modelled with good accuracy. Moreover, the presently available models require as input some properties of the fluids, such as the critical point pressure or the acentric factor, which could not be related directly to the surface tension values. Apart from this, they were constructed using only a small number of data for each fluid or data from just a single database as the only reference.

In this present work, we initially considered the database created by Cachadiña et al. [29], which includes data from different sources (Refs. [26–28] and papers published until 2014), updating it with the addition or replacement of new recently published data, as will be explained in Sec. 2.

As the main result, we propose a new correlation model that includes three adjustable coefficients obtained by a fitting procedure to the aforementioned data for 80 fluids. The results are presented and analysed in Sec. 3, where we include a comparison with the previous correlation models by Miqueu et al. [7], Di Nicola et al. [12,15] (two different models), and Gharagheizi et al. [11]. The conclusions are summarized in Sec. 4.

2. The new corresponding-states model

As usual, the procedure used to obtain a corresponding-states model is to define reduced variables for the surface tension and temperature, and then to propose an analytical relationship between them. Our proposal here is to include the values of the critical temperature T_c (at which the surface tension is zero by definition), and the surface tension and temperature at the normal boiling point, T_b and σ_b . We define these variables in a reduced (non-dimensional) form as follows:

$$T^* = (T_c - T)/(T_c - T_b)$$
(1)

$$\sigma^* = \sigma / \sigma_b \tag{2}$$

Both reduced properties, temperature T^* and surface tension σ^* , must be zero at the critical point and unity at the boiling point. This fact must be taken into account in order to posit an analytical relationship between the two properties.

It is clear that these reduced variables can only be calculated for those fluids for which the boiling temperature and surface tension values are known. Initially, we considered the database that we created in 2015 [29], which contains selected data for 86 refrigerants. We here update this database by considering the latest version of the DIPPR database (2016 version) [28], and adding or replacing new recently published data [30–33]. For four refrigerants (R225ca, R225 cb, R744-carbon dioxide, and R846-sulfur hexafluoride), a normal boiling point either cannot be defined (i.e., these fluids cannot boil at normal atmospheric pressure) or has not been measured. For two refrigerants (R114B2, and R1130), the data are unfortunately very disperse so that they do not follow any trend that can be adequately reproduced by a correlation model.

We have finally an up-to-date database that includes values for 80 refrigerants. We note that for 33 fluids the new version of DIPPR gives values that are different from those in the previous version used in Ref. [29]. For instance, for R10B1 the data included in the 2011 version disagreed with other values, and therefore no specific correlation was proposed in Ref. [29]. In the present version those values have been updated and they agree with other available values, so that it is now possible to fit them.

Apart from this, new published data have been added for 5 fluids. In particular, Cui et al. [30] give 7 new experimental data for R32, so these have also been added. In the case of R160, Cachadiña et al. [29] considered 14 data taken from DETHERM, but here 19 values are considered taken from both the DETHERM and the DIPPR databases [27,28]. We have added 43 new data for R161 published by Bi et al. [31], and 11 new data by Rausch et al. [32] for RE347mcc (or HFE-7000). Finally, for R1243zf, the values considered by Cachadiña et al. [29] have been replaced by 11 recent experimental data values given by Kondou et al. [33]. After these changes, the updated database used here contains 4067 data for 80 refrigerants.

Table 1 lists all the refrigerants considered, ordered by refrigerant number, including the number of data and the temperature range for which they are available, and values of the input properties used in our correlation model. The values T_c and T_b are those reported by DIPPR. Unfortunately, only for one fluid there is a data of the surface tension in our database obtained just at the T_b value given by DIPPR. Thus, the σ_b values in Table 1 are those calculated at T_b with a specific correlation that fits the data for each fluid by using the same analytical expression proposed by Cachadiña et al. [29] for each fluid, with updated values for the adjustable coefficients when needed. We note that for some fluids the boiling point temperature is outside the temperature range considered, so the σ_b values used in these cases are extrapolated ones.

For each fluid the reduced values (T^*, σ^*) were calculated by

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