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Corrigendum

Corrigendum to: “Combining the entropy-scaling concept and cubic- or SAFT equations of state for modelling thermal conductivity of pure fluids”

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The authors regret to report that, in their paper published in 2022 [1], they have identified an error in the calculation of the Tv-residual entropy using the *tc*-PR equation of state. We sincerely apologize for any caused inconvenience. For the sake of clarity, the mathematical expression of the *translated-consistent* Peng-Robinson (*tc*-PR) [2] cubic equation of state (EoS) and the corresponding correct formula for the Tv-residual entropy are given below.

For a pure component, the *tc*-PR equation writes:

$$P(T, v) = \frac{RT}{v + c_i - b_i} - \frac{a_i(T)}{(v + c_i)(v + c_i + b_i) + b_i(v + c_i - b_i)}$$

$$\left\{ \begin{array}{l} a_i(T) = a_{c,i} \alpha_i(T_r); T_r = \frac{T}{T_{c,i,\text{exp}}} \\ \alpha_i(T_r) = T_r^{N_i(M_i-1)} \exp[L_i(1 - T_r^{M_i N_i})] \\ c_i = v_{i,\text{liq}}^{\text{sat,u-PR}}(T_r = 0.8) - v_{i,\text{liq},\text{exp}}^{\text{sat}}(T_r = 0.8) \\ \eta_c = \left[1 + \sqrt[3]{4 - 2\sqrt{2}} + \sqrt[3]{4 + 2\sqrt{2}} \right]^{-1} \approx 0.25308 \\ a_{c,i} = \frac{40\eta_c + 8}{49 - 37\eta_c} \frac{R^2 T_{c,i,\text{exp}}^2}{P_{c,i,\text{exp}}} \approx 0.45724 \frac{R^2 T_{c,i,\text{exp}}^2}{P_{c,i,\text{exp}}} \\ b_i = \frac{\eta_c}{\eta_c + 3} \frac{RT_{c,i,\text{exp}}}{P_{c,i,\text{exp}}} \approx 0.07780 \frac{RT_{c,i,\text{exp}}}{P_{c,i,\text{exp}}} \end{array} \right. \quad (\text{C1})$$

Such a model is said *translated* [3,4] because a substance-dependent volume-translation parameter, c_i , is introduced, in order that the

translated EoS exactly reproduces the experimental saturated liquid volume at a reduced temperature of 0.8, [$v_{i,\text{liq},\text{exp}}^{\text{sat}}(T_r = 0.8)$]:

$$c_i = v_{i,\text{liq}}^{\text{sat,u-CEoS}}(T_r = 0.8) - v_{i,\text{liq},\text{exp}}^{\text{sat}}(T_r = 0.8) \quad (\text{C2})$$

where $v_{i,\text{liq}}^{\text{sat,u-CEoS}}(T_r = 0.8)$ is the molar volume calculated with the original (untranslated) EoS at $T_r = 0.8$. In turn, *consistent* stands for the fact that the *tc*-PR EoS relies on an α -function that passes the consistency test proposed by Le Guennec et al. [5,6]

Starting from Eq. (C1), the mathematical expression of the Tv-residual entropy can be straightforwardly determined by:

$$s_{Tv-\text{res}} = \left[\frac{\partial}{\partial T} \int_{\infty}^v \left(P(T, v) - \frac{RT}{v} \right) dv \right]_v$$

$$= R \ln \left(\frac{v + c_i - b_i}{v} \right) - \frac{1}{b_i(r_1 - r_2)} \ln \left(\frac{v + c_i - b_i r_1}{v + c_i - b_i r_2} \right) \cdot \underbrace{a_{c,i}}_{\text{omitted in 2022}} \frac{\partial \alpha_i}{\partial T} \quad (\text{C3})$$

$$\text{With: } \left\{ \begin{array}{l} r_1 = -1 - \sqrt{2} \\ r_2 = -1 + \sqrt{2} \\ \frac{\partial \alpha_i}{\partial T} = \frac{\alpha_i N_i}{T} (M_i - 1 - L_i M_i T_r^{M_i N_i}) \end{array} \right.$$

Unfortunately, in our paper from 2022, the $a_{c,i}$ quantity that appears in Eq. (C3) was involuntary omitted in our software leading to erroneous values of $s_{Tv-\text{res}}$.

Despite this regrettable error, the general conclusions and observations reported in our original article remain valid. After correcting this

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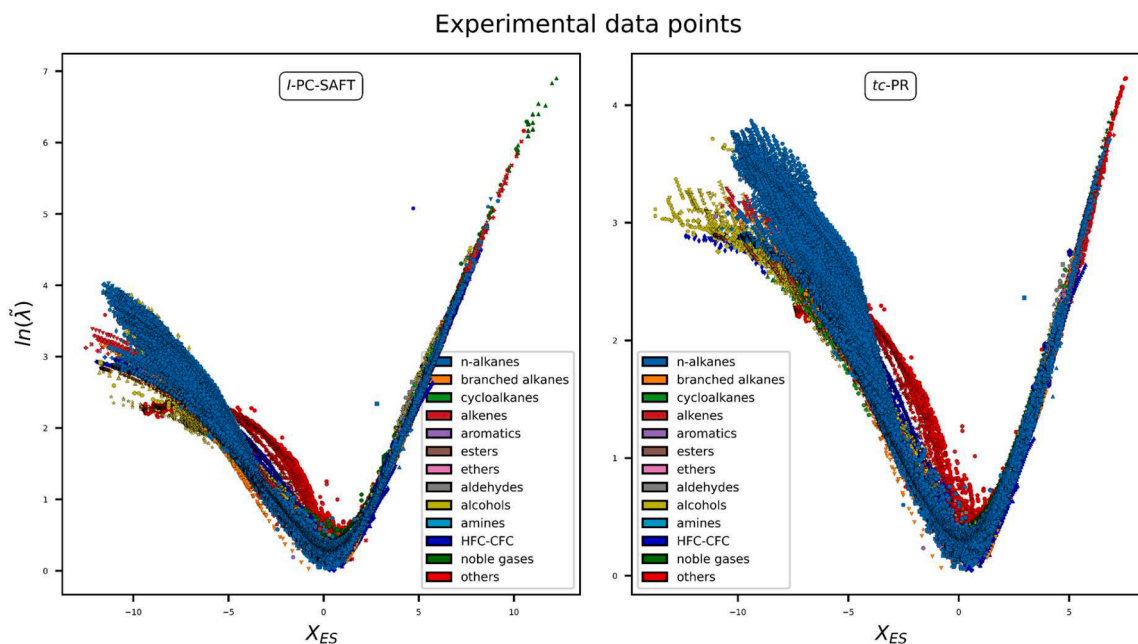


Fig. 5. Overview of all the experimental data in the $(\ln\tilde{\lambda}, X_{ES})$ plane. The thermodynamic properties involved in the calculation were estimated with the *I-PC-SAFT* EoS in the left subplot and with the *tc-PR* EoS in the right subplot. Each color corresponds to a chemical family and each symbol corresponds to a given chemical specie.

error, it was possible to conclude that the correction introduced at high temperatures for light molecules was no longer necessary when the *tc-PR* EoS was used. As a result, exactly the same formalism is now used for both the *I-PC-SAFT* and *tc-PR* EoS. This is a positive point. A more detailed analysis of results shows that by using component-specific parameters, the results remain excellent with a global average deviation around 4%. When chemical-family specific parameters are used, the overall mean deviation rises from 5.6% to 10.1%, becoming comparable to that obtained with the *I-PC-SAFT* EoS. This increase is due to a poorer correlation of hydrocarbons when using chemical-family parameters. By using universal parameters, the average deviation on our complete database increases slightly and the deviations obtained with the *tc-PR* EoS (around 12%) become comparable to those obtained with the *I-PC-SAFT* EoS (around 11%).

Clearly, the numerical values of the coefficients to be used in the developed correlations when the *tc-PR* EoS is considered have to be updated. All results related to the *I-PC-SAFT* EoS [7] are unaltered by our error.

Corrigendum to the Supplementary Material: all fitted coefficients related to the *tc-PR* EoS based model are now updated in the new version of the supplementary material that was built with the correct values of s_{TV-res} .

Corrigendum to section 2.3: the section “Our paper devoted to viscosity underlined that numerical values of s_{TV-res} could differ significantly from one EoS to another. Although dividing the *Tv-residual entropy* by its value at the critical point strongly attenuates this difference, we found necessary to add a temperature-dependent term in the mathematical expression of the X_{ES} variable (see Eq. (11)) when the *tc-PR* EoS is used. This patch, specific to the *tc-PR* EoS and only needed at very high temperatures ($4T_c < T < 8T_c$, where T_c denotes the critical temperature of the fluid) was introduced to keep the same mathematical expression of the X_{ES} variable (see Eq. (10)) regardless of the EoS used to estimate the density, residual isochoric heat capacity and residual entropy: it is indeed enough to select $f_{corr}(T) = 1$ in Eq. (11) when one works with the *I-PC-SAFT* EoS. To sum up, for heavy molecules for which the temperature domain $T > 4T_c$ is not of practical

interest, a null α value is selected in Eq. (11). Otherwise, for light molecules (having a low T_c) such as Ar, N_2 or Krypton for which experimental thermal conductivities are available at high reduced temperatures ($4T_c < T < 8T_c$) a non-zero coefficient was selected. The influence of this correction is illustrated with Argon in Fig. 16 of Appendix A. It is worth noting that as long as a given equation of state qualitatively reproduces the temperature and pressure dependence of the *Tv-residual entropy* regardless of the fluid conditions (as the *I-PC-SAFT* EoS does), it is not necessary to apply this patch”, including (Eq. 11) of our original article, should be discarded since the concerned phenomenon is considerably reduced and becomes negligible when using the correct values of s_{TV-res} . In other words, after correcting the *Tv-residual entropy* values, it was found that $f_{corr}(T) = 1$ was also suitable for the *tc-PR* EoS.

Corrigendum to equation 16: with the correct values of the residual entropy returned by the *tc-PR* EoS, the authors found it unnecessary to modify the X_{ES} formulation for high temperatures and thus the same X_{ES} as for the *I-PC-SAFT* EoS should be used for the *tc-PR* EoS. Therefore, (Eq. 16) should be corrected as follows.

$$\left\{ \begin{array}{l} \ln\left(\frac{\lambda}{\lambda_{ref}^{Rosenfeld, \text{intDoF}}}\right)_{calc} = \left[\left(\frac{a_1 + a_2 X_{ES}^{1/3}}{1 + e^{X_{ES}}} \right) + \left(\frac{b_1 + b_2 X_{ES}^{1/3}}{1 + e^{-X_{ES}}} \right) \right] X_{ES} + d \\ \lambda_{ref}^{Rosenfeld, \text{intDoF}} = \rho_N^{2/3} k_b \sqrt{\frac{k_b T}{m_0}} \left[1 + \left(\frac{c_v^{real}}{R} \right) e^{-(\rho/\rho_c)} \right] \\ X_{ES} = \left(-\frac{\tilde{s}_{TV-res}}{\tilde{s}_c} \right) - \ln\left(\frac{\tilde{s}_{TV-res}}{\tilde{s}_c}\right) \text{ for both } I-PC-SAFT \text{ and } tc-PR \text{ EoS} \end{array} \right. \quad (16)$$

Corrigendum to the overall MAPEs obtained using the *tc-PR* EoS: the overall MAPEs were 3.38%, 5.57% and 9.19% for the component-specific, the chemical-family specific and the universal parameters respectively. They are now 4.28%, 10.09% and 12.28% respectively after using the correct values of the *Tv-residual entropy*.

Corrigendum to Appendix A: the correction that was originally proposed to counteract some undesired behavior at high temperatures is

tc-PR - component-specific parameters

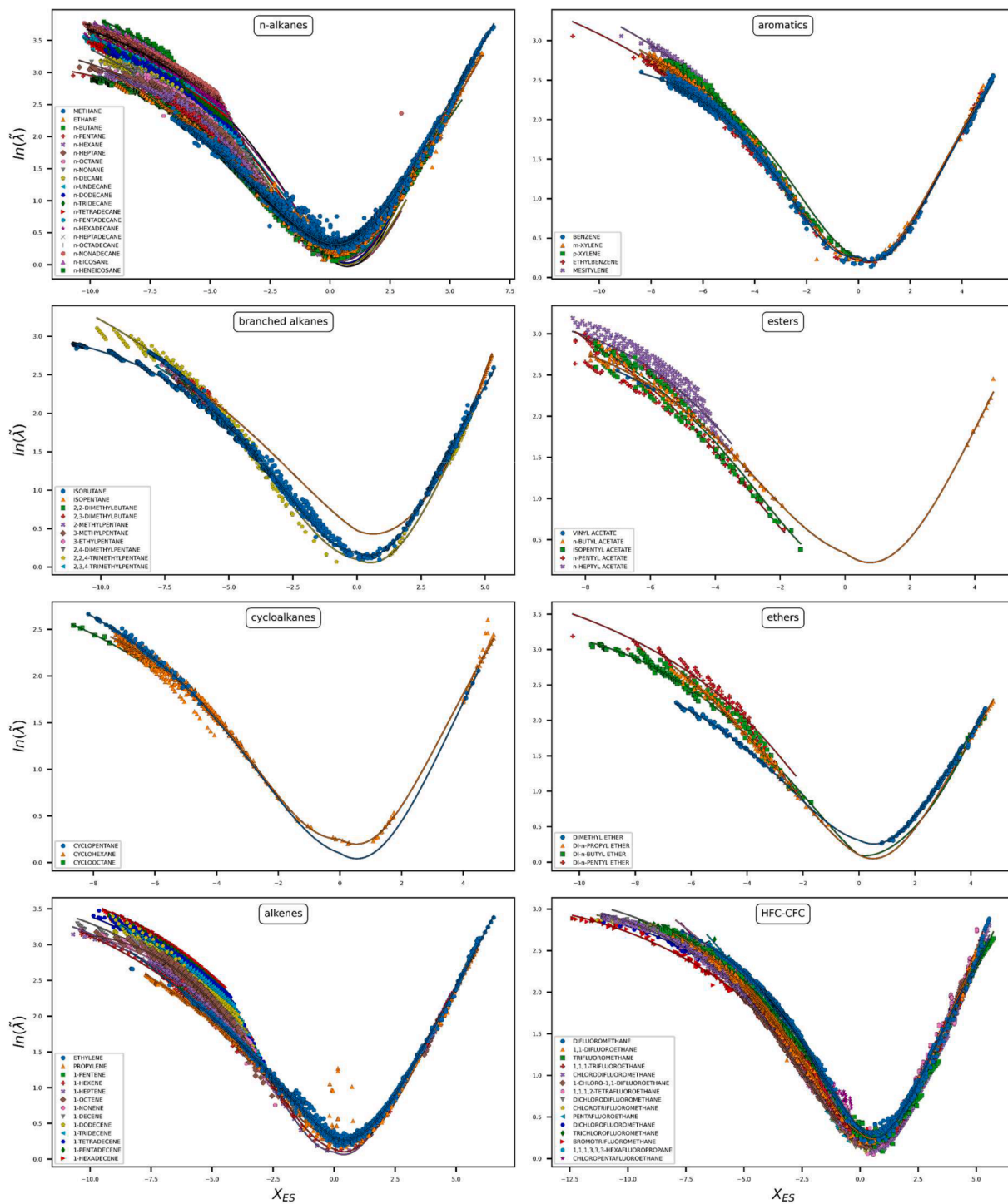


Fig. 7. Results of the combination of the component-specific parameters with the *tc*-PR EoS for modelling the thermal conductivity of n-alkanes, branched alkanes, cycloalkanes, alkenes, aromatics, esters, ethers and HFC-CFCs. Symbols represent the experimental data points; Solid lines represent the calculated values.

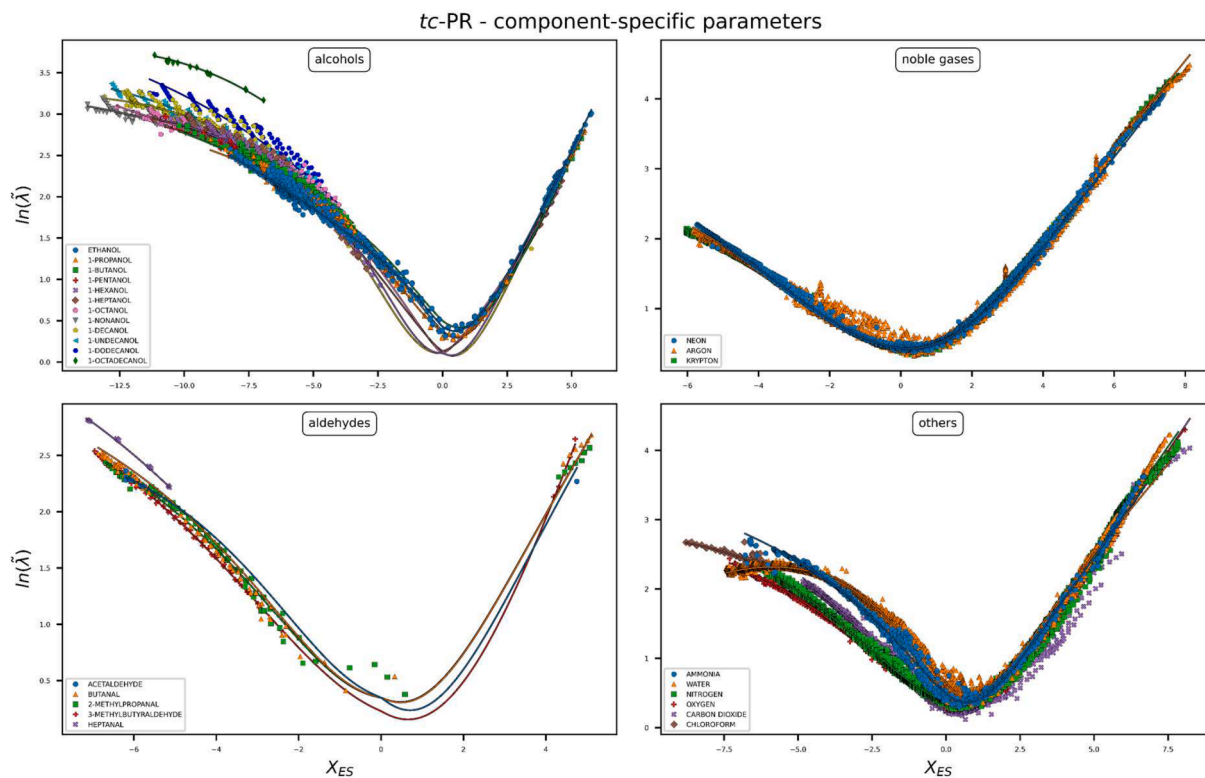


Fig. 9. Results of the combination of the component-specific parameters with the *tc*-PR EoS for modelling the thermal conductivity of alcohols, noble gases, aldehydes and other chemical species. Symbols represent the experimental data points; Solid lines represent the calculated values.

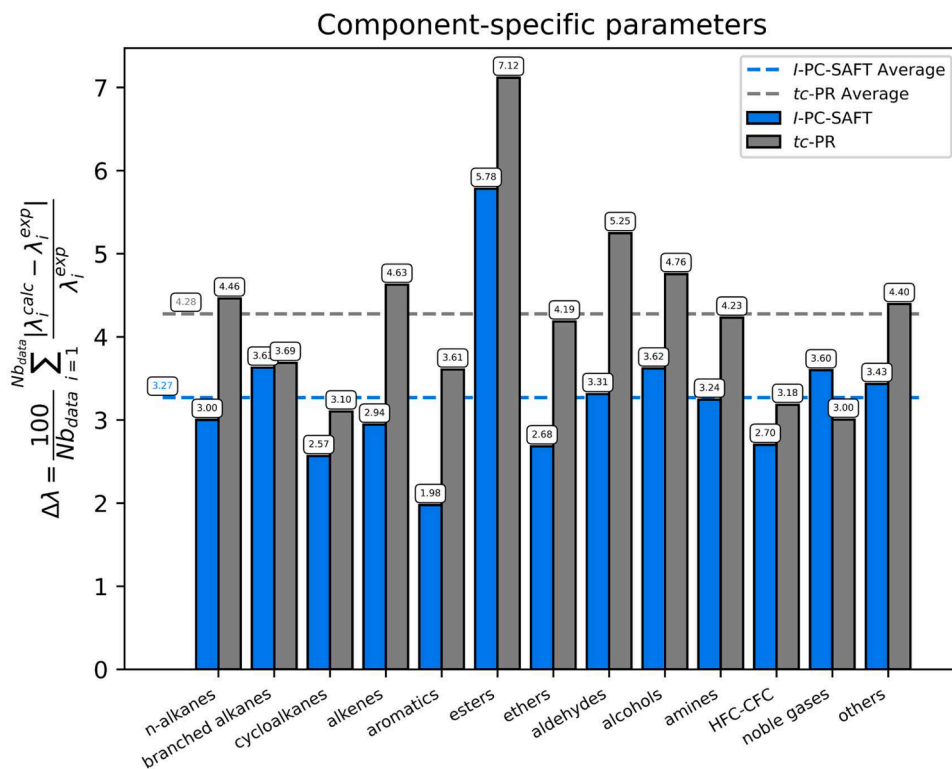


Fig. 10. Summary of MAPEs obtained with the *I*-PC-SAFT and the *tc*-PR EoS in combination with the component-specific parameters.

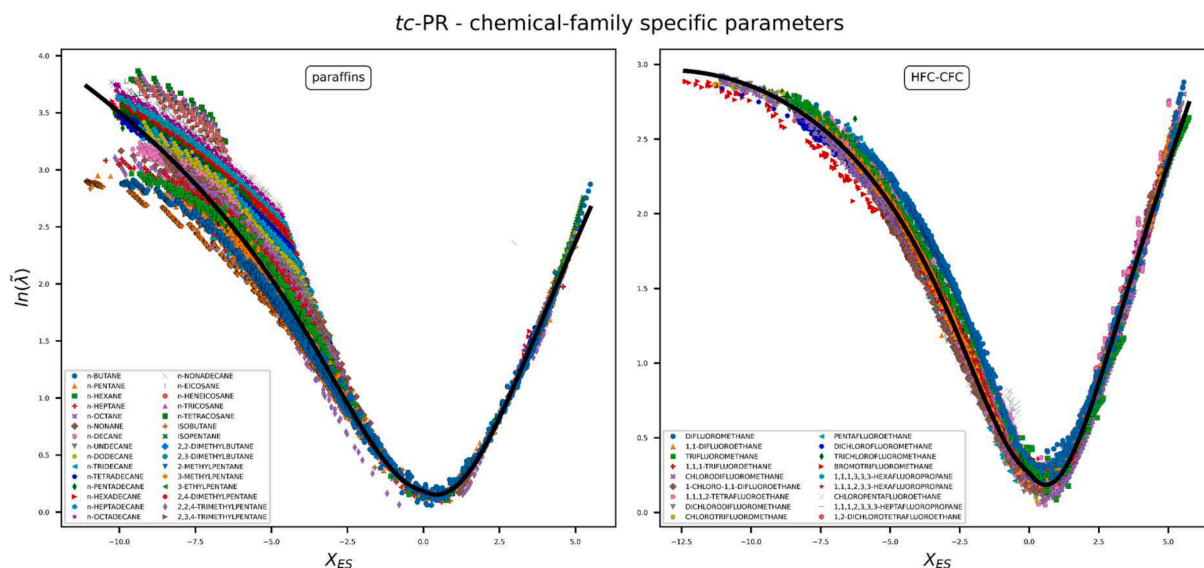


Fig. 12. Results of the combination of the chemical-family specific parameters with the *tc*-PR EoS for modelling the thermal conductivity of paraffins and HFC-CFCs. Symbols represent the experimental data points; Solid lines represent the calculated values.

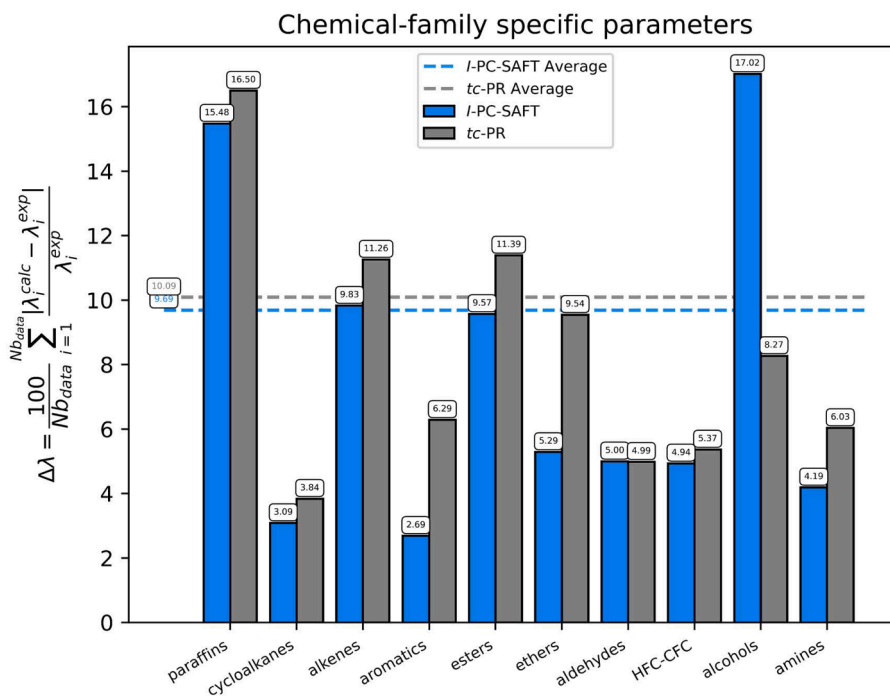


Fig. 13. Summary of MAPEs obtained with the *I*-PC-SAFT and the *tc*-PR EoS in combination with the chemical-family specific parameters.

now discarded due to the phenomenon becoming negligible while using the correct values of the *T_v*-residual entropy. Therefore, the appendix A which contains Fig. 16 should be discarded.

Corrigendum to Figs 5, 7, 9, 10, 12, 13, 14, 15: after the correction of the *T_v*-residual entropy values, involved in the *X_{ES}* variable, the figures reporting the results of the *tc*-PR EoS are updated as follows.

CRediT authorship contribution statement

Aghilas Dehlouz: Conceptualization. **Jean-Noël Jaubert:** Writing –

review & editing. **Guillaume Galliero:** Supervision. **Marc Bonnissel:** Resources. **Romain Privat:** Writing – review & editing.

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.

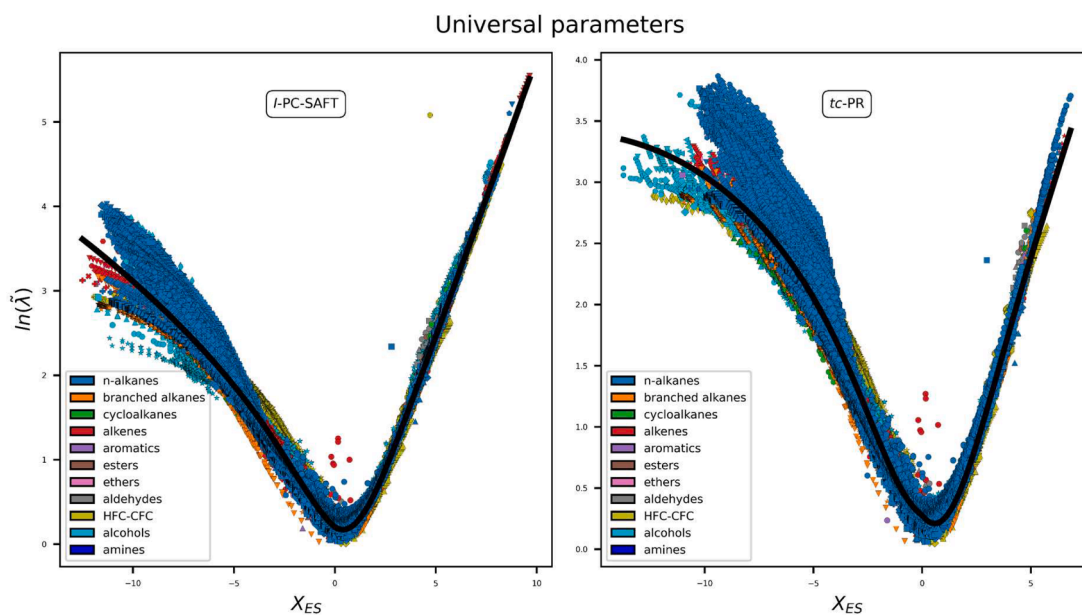


Fig. 14. Results of the combination of the universal parameters with the *I*-PC-SAFT and the *tc*-PR EoS for modelling the thermal conductivity. Each color corresponds to a chemical family and each symbol correspond to a given chemical specie; Solid lines represent the calculated values.

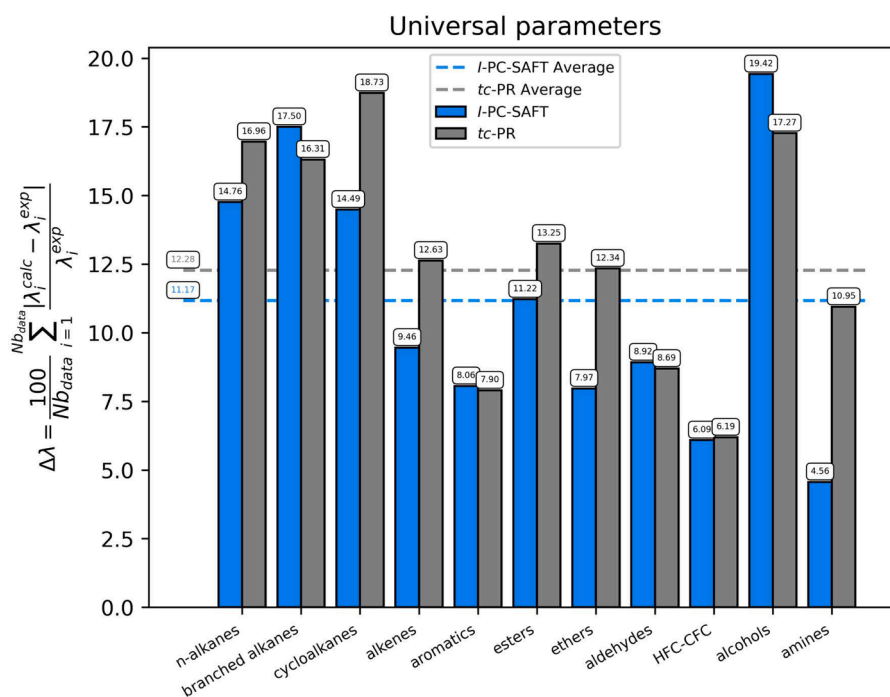


Fig. 15. Summary of MAPEs obtained with the *I*-PC-SAFT and the *tc*-PR EoS in combination with the universal parameters.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.ijheatmasstransfer.2024.126121](https://doi.org/10.1016/j.ijheatmasstransfer.2024.126121).

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