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# Corrigendum to: “Entropy Scaling-Based Correlation for Estimating the Self-Diffusion Coefficients of Pure Fluids”

Aghilas Dehlouz, Jean-Noël Jaubert,\* Guillaume Galliero, Marc Bonnissel, and Romain Privat\*

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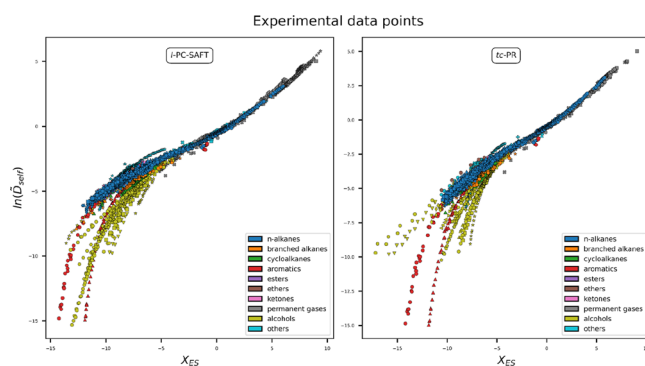
Article Recommendations

Supporting Information

The authors regret to report that they have identified two errors in the Fortran code that they wrote and was used to generate the results they published in 2022.<sup>1</sup>

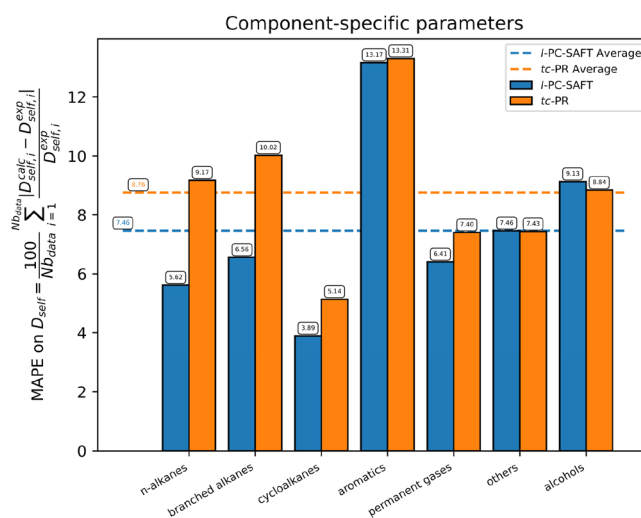
**Table 2. Universal Parameters for the Self-Diffusion Model in the Dilute Gas Region ( $X_{ES} \geq 0$ ) Associated with Two Different EoS (Used for Estimating Density and Residual Entropy), Namely, the *I*-PC-SAFT and *tc*-PR Models**

EoS	<i>I</i> -PC-SAFT	<i>tc</i> -PR
$b_{univ}$	0.6686	0.6621
$c_{univ}$	0.2861	0.3351
$d_{univ}$	−0.5451	−0.5969



**Figure 4.** Overview of all experimental data in the  $\ln(\tilde{D}_{self})$  vs  $X_{ES}$  plane. The thermodynamic properties involved in the definition of  $\tilde{D}_{self}$  and  $X_{ES}$  were estimated using the *I*-PC-SAFT EoS (left panel) and the *tc*-PR EoS (right panel). Each color corresponds to a specific chemical family, and each symbol corresponds to a specific compound.

- The first error was a mistake in reading the experimental data file, which led to only one experimental data point out of 2 being considered. Consequently, the deviations reported in 2022, between experimental and calculated self-diffusion coefficients only considered half of the available data points. [Table S1 of the Supporting Information](#), attached to this corrigendum, provides detailed information on the data considered in this study.
- The second error was in the equation used to calculate the  $T_v$ -residual entropy from the *translated-consistent* Peng–Robinson (*tc*-PR)<sup>2</sup> cubic equation of state (EoS).



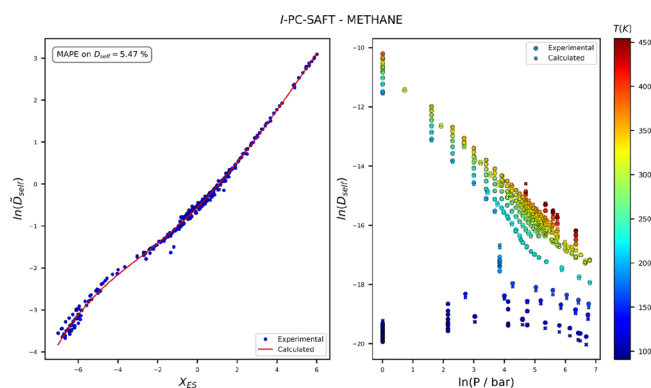
**Figure 5.** Correlation of self-diffusion coefficients using the model given by eq C4 and parametrization strategy 1 (component-specific parameters). Summary of the MAPEs obtained using either the *I*-PC-SAFT or the *tc*-PR EoS for estimating density and residual entropy.

The authors sincerely apologize for the inconvenience caused and, in order to clarify the second error, have decided to recall below the correct equation to be used to calculate the  $T_v$ -residual entropy from the *tc*-PR EoS.

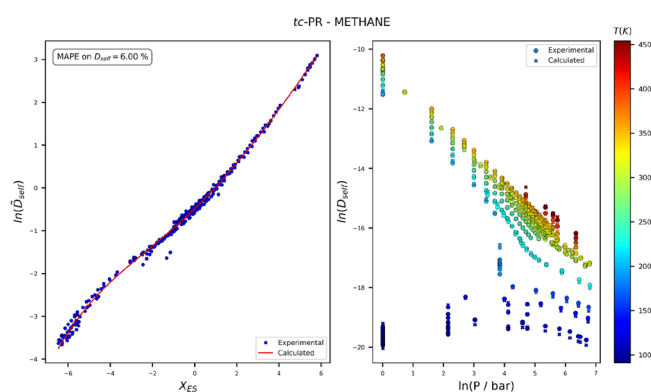
For a pure component, the *tc*-PR equation writes:

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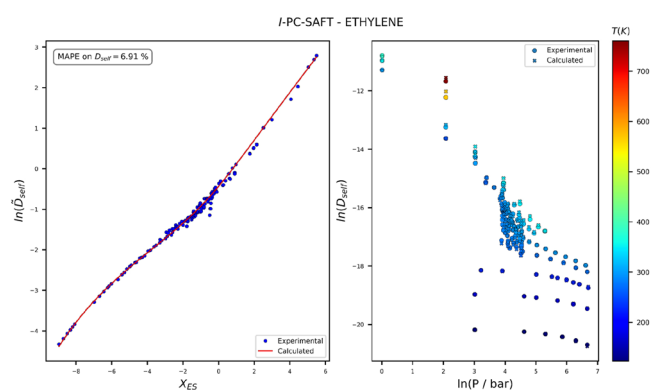




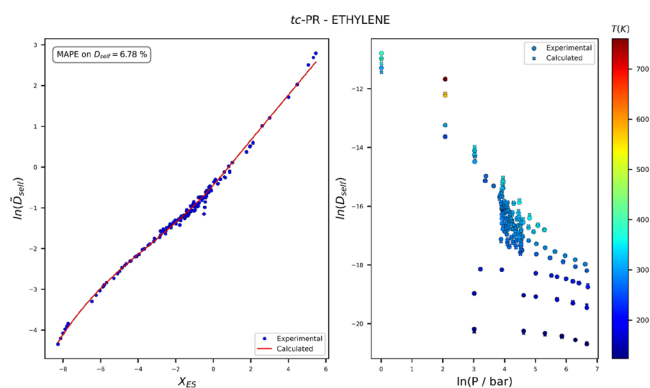
**Figure 6.** Application of the entropy scaling (ES)-based model combining eq C4 and parametrization strategy 1 to methane using the *I*-PC-SAFT EoS to estimate density and residual entropy. Left panel:  $(X_{ES}, Y_{ES})$  plane. Right panel: self-diffusion coefficient vs pressure (log–log scale).



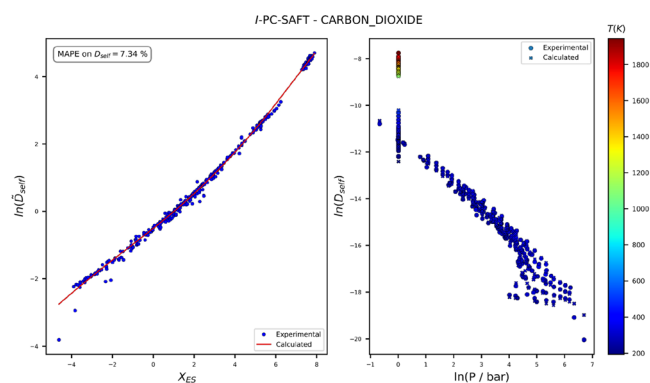
**Figure 7.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to methane using the *tc*-PR EoS (for more details, refer to the caption of Figure 6).



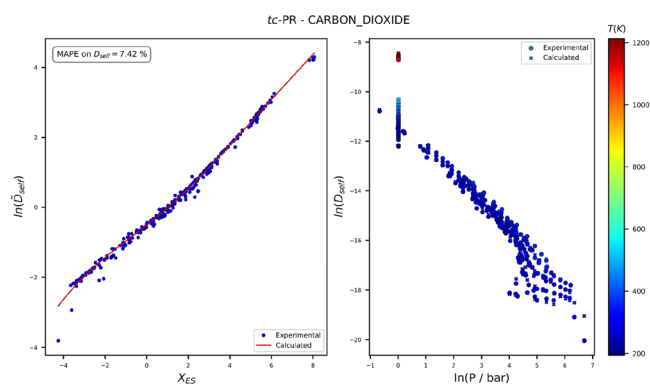
**Figure 8.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to ethylene using the *I*-PC-SAFT EoS (for more details, refer to the caption of Figure 6).



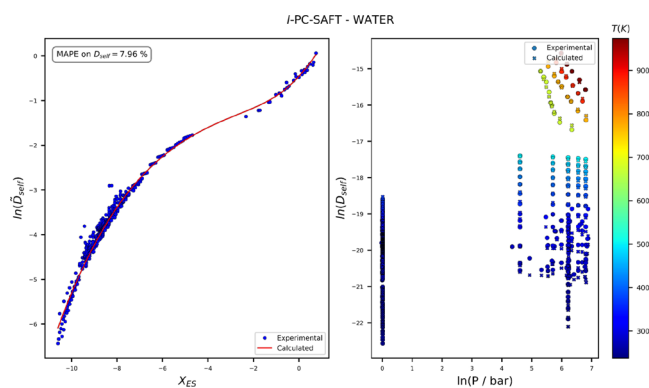
**Figure 9.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to ethylene using the *tc*-PR EoS (for more details, refer to the caption of Figure 6).



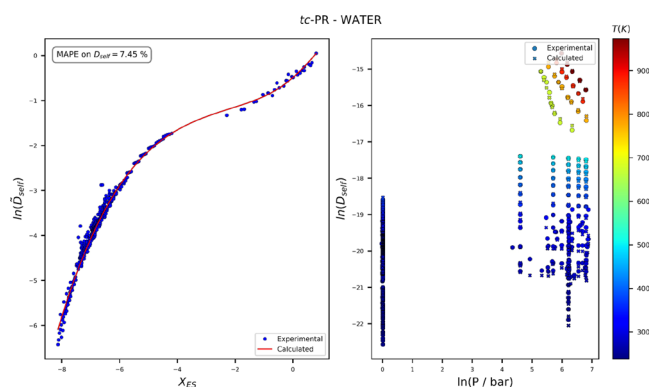
**Figure 10.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to CO<sub>2</sub> using the *I*-PC-SAFT EoS (for more details, refer to the caption of Figure 6).



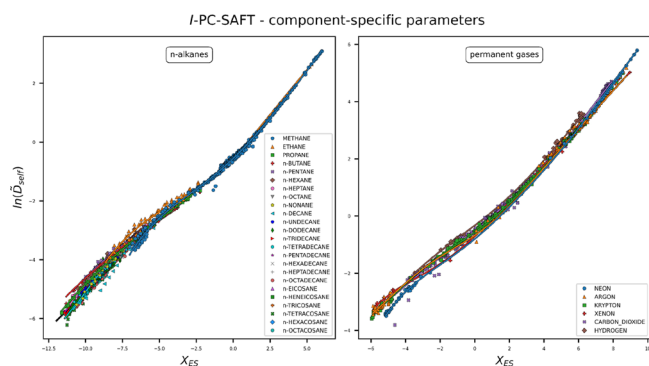
**Figure 11.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to CO<sub>2</sub> using the *tc*-PR EoS (for more details, refer to the caption of Figure 6).



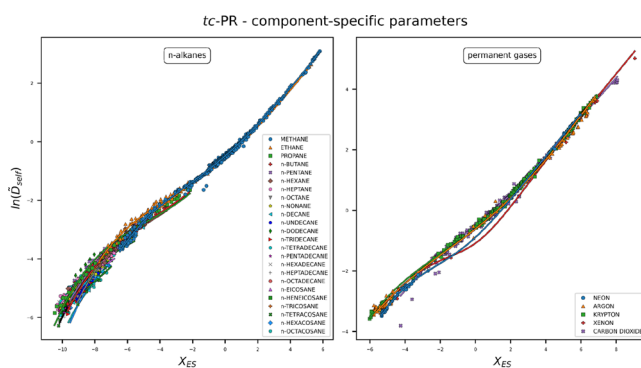
**Figure 12.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to water using the *I*-PC-SAFT EoS (for more details, refer to the caption of Figure 6).



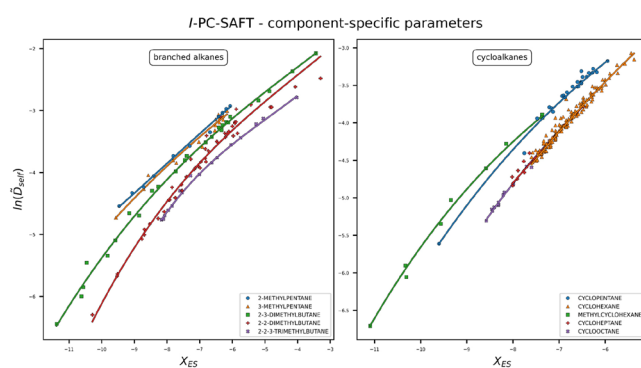
**Figure 13.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to water using the *tc*-PR EoS (for more details, refer to the caption of Figure 6).



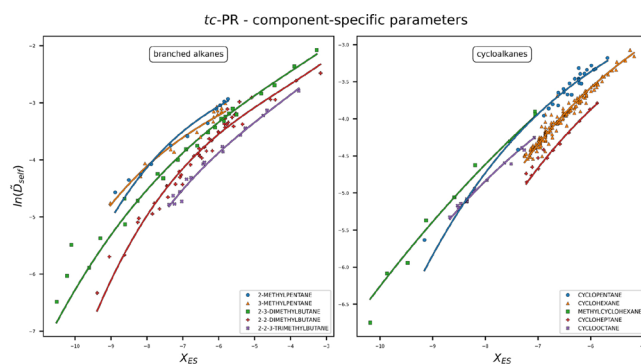
**Figure 14.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to *n*-alkanes and permanent gases using the *I*-PC-SAFT EoS. Points represent experimental data; solid line represents model data.



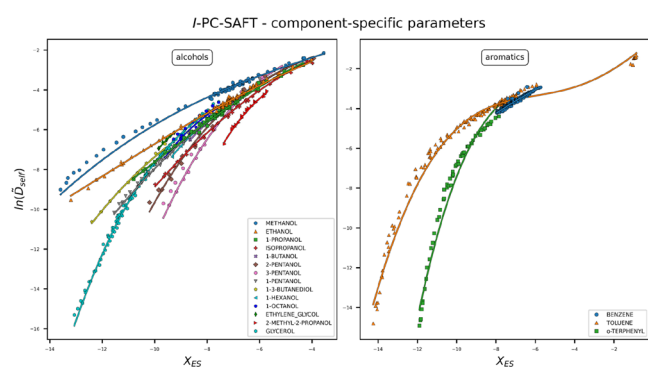
**Figure 15.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to *n*-alkanes and permanent gases using the *tc*-PR EoS. Points represent experimental data; solid line represents model data.



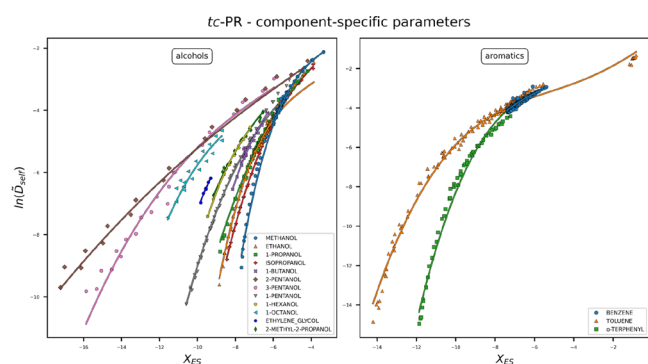
**Figure 16.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to branched alkanes and cycloalkanes using the *I*-PC-SAFT EoS. Points represent experimental data; solid line represents model data.



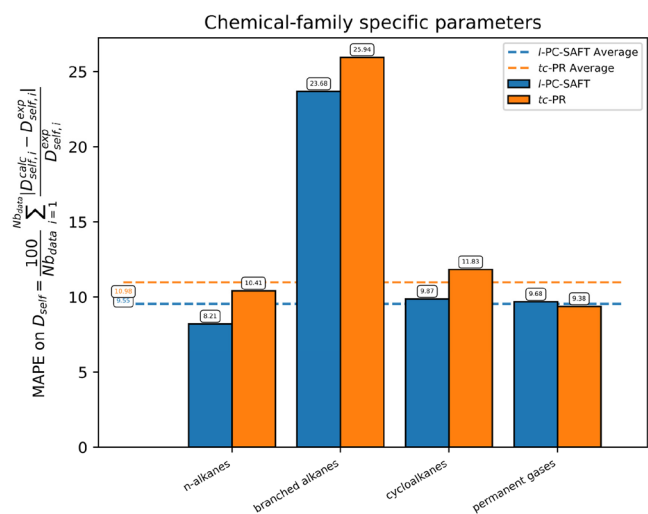
**Figure 17.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to branched alkanes and cycloalkanes using the *tc*-PR EoS. Points represent experimental data; solid line represents model data.



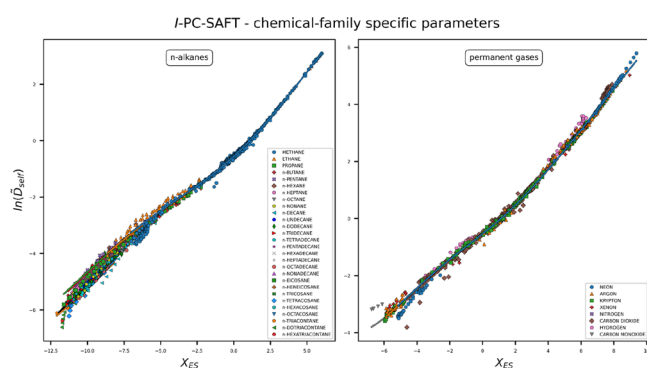
**Figure 18.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to *n*-alcohols and aromatic compounds using the *I*-PC-SAFT EoS. Points represent experimental data; solid line represents model data.



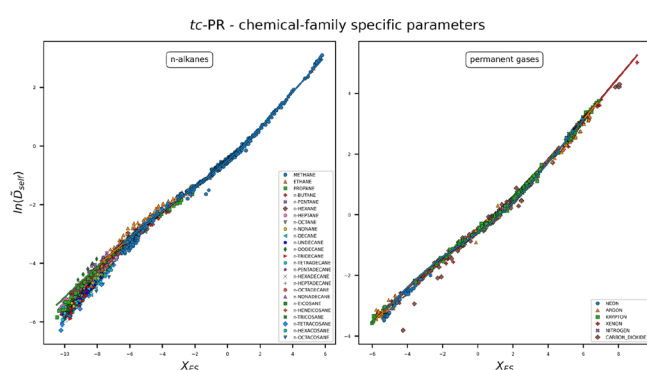
**Figure 19.** Application of the ES-based model combining eq C4 and parametrization strategy 1 to *n*-alcohols and aromatic compounds using the *tc*-PR EoS. Points represent experimental data; solid line represents model data.



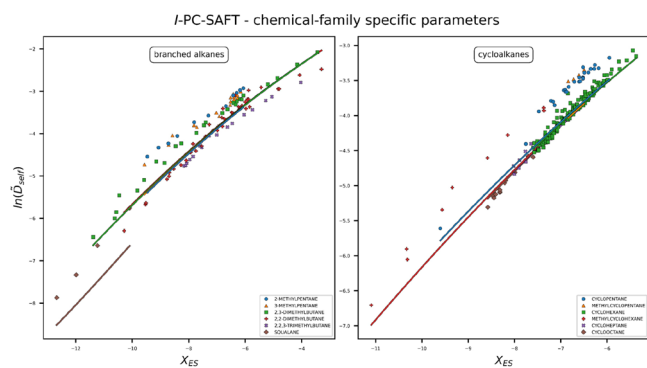
**Figure 20.** Prediction of self-diffusion coefficients using the model given by eq C4 and parametrization strategy 2 (with chemical-family specific parameters). Summary of the MAPEs obtained using either the *I*-PC-SAFT or the *tc*-PR EoS for estimating density and residual entropy.



**Figure 21.** Application of the ES-based model combining eq C4 and parametrization strategy 2 to *n*-alkanes and permanent gases using the *I*-PC-SAFT EoS. Points represent experimental data; solid line represents model data.



**Figure 22.** Application of the ES-based model combining eq C4 and parametrization strategy 2 to *n*-alkanes and permanent gases using the *tc*-PR EoS. Points represent experimental data; solid line represents model data.



**Figure 23.** Application of the ES-based model combining eq C4 and parametrization strategy 2 to aromatic compounds and ketones using the *I*-PC-SAFT EoS. Points represent experimental data; solid line represents model data.



whereas the term “parametrization strategy 2” means that chemical-family specific parameters are used.

## ■ ASSOCIATED CONTENT

### SI Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.iecr.4c02704>.

Presentation of the experimental database used for the ES-based correlation development; parameters to be used with the *I*-PC-SAFT-based model; parameters to be used with the *tc*-PR-based model (PDF)

Deviations between calculated and experimental self-diffusion coefficients for the experimental data points used in this study (XLSX)

## ■ ACKNOWLEDGMENTS

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