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Addition/Correction

Erratum for "Model Performances Evaluated for Infinite Dilution Activity Coefficients Prediction at 298.15 K"

Thomas Brouwer and Boelo Schuur*

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This erratum to our manuscript is prepared in response to feedback from readers of our paper 10.1021/acs.iecr.9b06238. We were correctly notified that, in the complilation of the infinite diluted activity coefficient database that is used in this work, and the predicted values of various models, a few errors were made. Upon inspection of the 5194 evaluated binary mixtures, we found 24 entries for infinite dilution activity coefficients with errors. In 18 out of the 24 cases, iodomethane was incorrectly used instead of diiodomethane, while the other 6 cases involved an incorrect placement of the decimal sign, which resulted in erroneous experimental infinite diluted activity coefficients.

Furthermore, upon carefully checking the data and the article, we found that the *y*-axis scale in Figure 2B was wrong, as it was based on a fraction and not on a percentage. This is merely a graphical error; in the tables and discussions, the correct values have been used. With this erratum document, we would like to correct these errors in the article and electronic Supporting Information (ESI). The corrected values can be found in the revised Supporting Information highlighted in yellow (pp 79, 81, 83, 84, 87, 88, 121, 172, and 179).

Overall, the 24 actual data errors in the infinite dilution activity coefficients have led to a minor implication in the calculations on the model prediction accuracies. The comparison between the original reported values and the new ones is presented in Table E1, and the differences are discussed in the text below (Table E1).

Table E1. Comparison of the Original and Corrected Values of the Average Relative Deviations Corresponding to Figure 2 from the Original Article and Figure E1 (Corrected)

	original ARD	corrected ARD
Hildebrand	$2.41 \times 10^5 \pm 4.77 \times 10^5$%	$2.41 \times 10^5 \pm 4.77 \times 10^5$%
HSP	66.4 ± 14.4%	66.4 ± 14.4%
modified UNIFAC(Ly)	32.2 ± 1.8%	32.0 ± 1.8%
UNIFAC	31.1 ± 1.7%	30.8 ± 1.7%
COSMO-RS	28.3 ± 1.1%	28.2 ± 1.1%
modified UNIFAC(Do)	24.3 ± 1.6%	24.0 ± 1.6%
Abraham	21.7 ± 1.2%	21.6 ± 1.2%
MOSCED	16.2 ± 1.3%	16.1 ± 1.3%

Table E2. Original and Corrected Values Corresponding with Table 1 in the Original Article

model	solvent	solute	original ARD (%)	corrected ARD (%)	difference (%)
MOSCED	halogen	aliphatic	18.1	12.3	5.8
	halogen	aromatic	9.8	5,.5	4.3
	aprotic	aliphatic	15.7	15.3	0.4
	aprotic	halogen	15.8	16.2	−0.4
Abraham	halogen	aliphatic	34.6	34.0	0.6
	aprotic	aliphatic	21.2	21.1	0.1
COSMO-RS	aromatic	halogen	26.7	27.4	0.7
	halogen	aliphatic	27.6	27.3	0.3
	halogen	aromatic	36.6	36.9	0.3
	halogen	halogen	15.7	16.6	−0.3
	aprotic	aliphatic	32.7	32.5	0.2
	aprotic	halogen	32.5	33.1	−0.6
UNIFAC	aromatic	halogen	20.9	19.9	1.0
	halogen	aliphatic	34.8	32.4	2.4
	halogen	halogen	19.4	18.7	0.7
	halogen	aprotic	18.0	17.2	0.8
	aprotic	aliphatic	40.3	40.1	0.2
	aprotic	halogen	23.0	24.0	−1.0
mod. UNIFAC (Ly)	halogen	aliphatic	34.0	31.1	2.9
	halogen	halogen	24.7	23.7	1.0
	halogen	aprotic	19.9	19.8	0.1
	aprotic	aliphatic	41.0	40.7	0.3
	aprotic	halogen	23.7	24.1	−0.4
mod. UNIFAC (Do)	aromatic	halogen	17.1	17.2	−0.1
	halogen	aliphatic	32.0	28.5	3.5
	halogen	halogen	13.5	12.2	1.3
	halogen	aprotic	17.5	17.4	0.1
	aprotic	aliphatic	30.1	29.8	0.3
	aprotic	halogen	25.9	27.1	−1.2

As can be seen in Table E1, the differences are very minor and always within the error margins.

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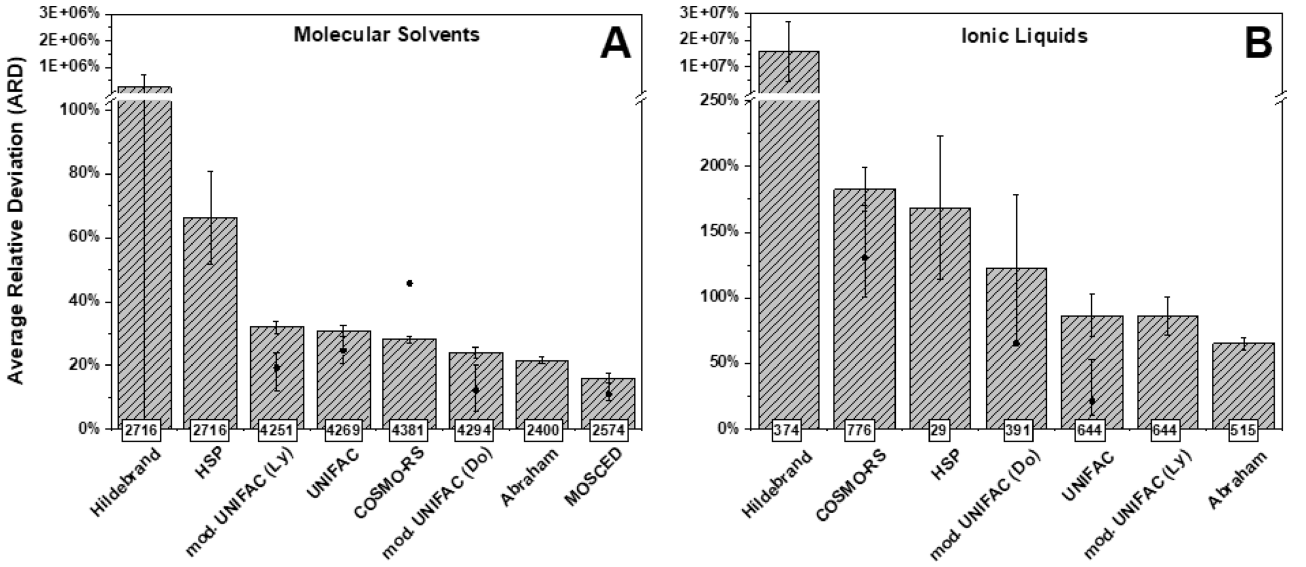

Figure E1. Evaluation of various predictive models for γ_i^{∞} for (A) molecular solvents and (B) ionic liquids (ILs) at 298.15 K. On the *y*-axis, the ARD is presented within the boxes the total amount of comparisons made. The experimental γ_i^{∞} is collected in the ESI. The integrated scatter plot depicts similar comparison made in the literature for various models, e.g., modified UNIFAC(Ly),[17−19] UNIFAC,[17−22,42,43] COSMO-RS,[18,44] modified UNIFAC(Do),[17,19,22,23,45−47] and MOSCED.[6,20−22,24]

The adjusted Figure 2 from the main manuscript is shown below in Figure E1. A new *y*-axis is used for panel (B) in the original Figure 2; the scale is 100 times greater than the old one.

In the more detailed analysis within specific binary couples of molecular solvents (Table 1 in the main manuscript), minor changes in accuracy also occurred, as can be seen in Table E2.

This results in a single change in the overview of the most accurate predictive model of molecular solvents seen in Table 4 of the original article, where the Abraham model (original: 16.1%, corrected: 16.1%) is now more accurate for the halogen−halogen combination than the COSMO-RS model (original: 15.7%, corrected: 16.6%).

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.iecr.3c00757.

The ESI supports the main manuscript with all the specific parameters, equations and predictions for the various models. Also all the experimental used in the comparison are attached with the corresponding references (PDF)

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