Comparison of S5P/TROPOMI inferred NO_2 surface concentrations with in-situ measurements over Central Europe

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Introduction

In this work, NO_2 surface concentrations inferred from the S5P/TROPOMI instrument are evaluated over Central Europe for the summer of 2019 and the winter of 2019/2020. Simulations of the NO_2 VCDs and surface concentrations from the LOTOS-EUROS v2.02.001 CTM are also applied in the methodology. The derived TROPOMI NO_2 surface concentrations are examined further with the altering of three major influencing factors: i) the vertical levelling scheme of the model, ii) the TROPOMI NO_2 data version and iii) the AMFs and AKs applied to the satellite and modelled NO_2 VCDs and surface concentrations. The TROPOMI derived NO_2 surface concentrations are then compared with more than two hundred ground-based stations reporting to the EEA database.

Study domain and Methodology

Figure 1. Study domain [red box] and ground-based stations locations [green boxes]. Stations are separated into 7 types: urban and suburban traffic, urban, suburban and rural background and suburban and rural industrial.

S5P/TROPOMI inferred NO_2 surface concentration evaluation

$$S_O = (\Omega_O/\Omega_G) * S_G$$

S: NO_2 surface concentration
Ω: NO_2 vertical column density
O: Satellite observations
G: Model simulations

Updated AMFs and AKs

Estimation of alternative tropospheric AMFs and AKs based on the LOTOS-EUROS a priori profiles instead of the TM5-MP profiles.

Setups	LOTOS-EUROS	TROPOMI
Setup 1	A priori S_G and Ω_G	A priori Ω_O
Setup 2	TM5-MP AKs on S_G and Ω_G	A priori Ω_O
Setup 3	A priori S_G, Ω_G with updated AMFs and AKs	Ω_O with updated AMFs and AKs

Table 1. Datasets and their products involved in each setup in order to estimate TROPOMI inferred NO_2 surface concentrations.

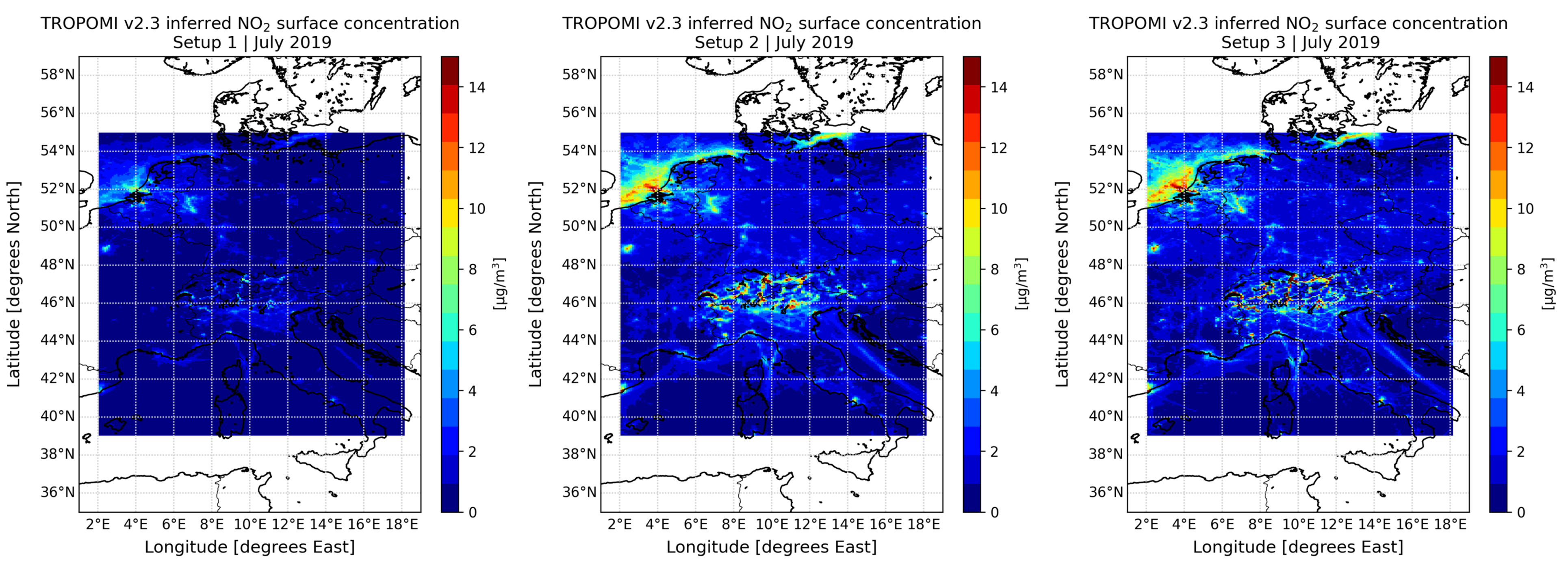

Figure 2. TROPOMI v2.3 inferred NO_2 surface concentrations for July 2019 for the 1st [left], the 2nd [middle] and the 3rd [right] setups. It is evident that as we move from the case of not applying AKs [left], to applying the original TROPOMI TM5-MP AKs [middle] and to applying the updated AKs [left], the inferred NO_2 surface concentration increases. Note that road transport and shipping tracks are more pronounced in the third setup, especially in the Po valley and the Adriatic Sea. Concentrations are higher by **3%** and **72%** in the 3rd setup for those regions when compared to the 2nd and the 1st setups, respectively.

Effect of the LOTOS-EUROS vertical levelling scheme

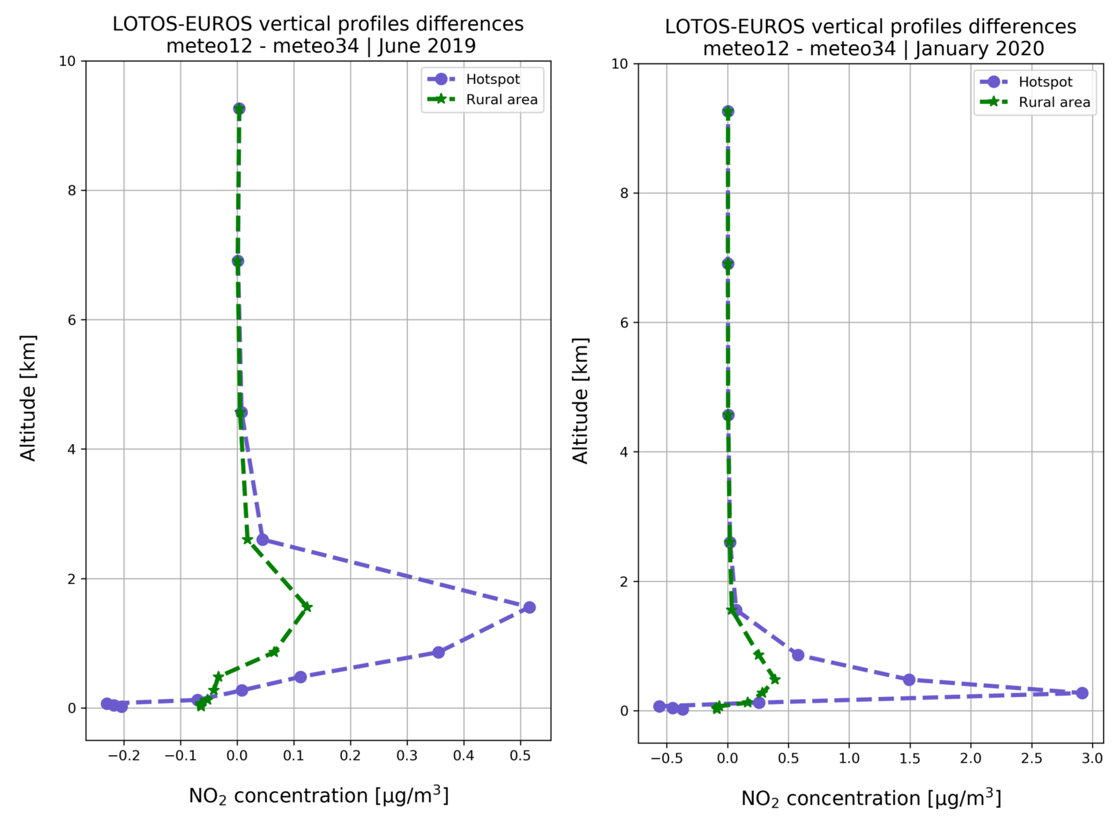

Figure 3. Meteo12 and meteo34 profiles differences for June 2019 [left] and January 2020 [right] for a hotspot [purple] and a rural [green] pixels in the city of Amsterdam. Both hotspot and rural pixels are selected as the closest to a traffic and a rural stations. In both summer and winter, the meteo34 scheme shows higher concentrations for the first 3 layers. Meteo12 shows higher NO_2 concentrations between the fifth and the ninth layer while for higher layers the differences become negligible.

LOTOS-EUROS vertical levelling schemes	
meteo12	12 coarsened vertical layers up to 9 km
meteo34	34 vertical layers up to 30 km, same vertical structure with the ECMWF data

Table 2. LOTOS-EUROS vertical levelling schemes used in this study.

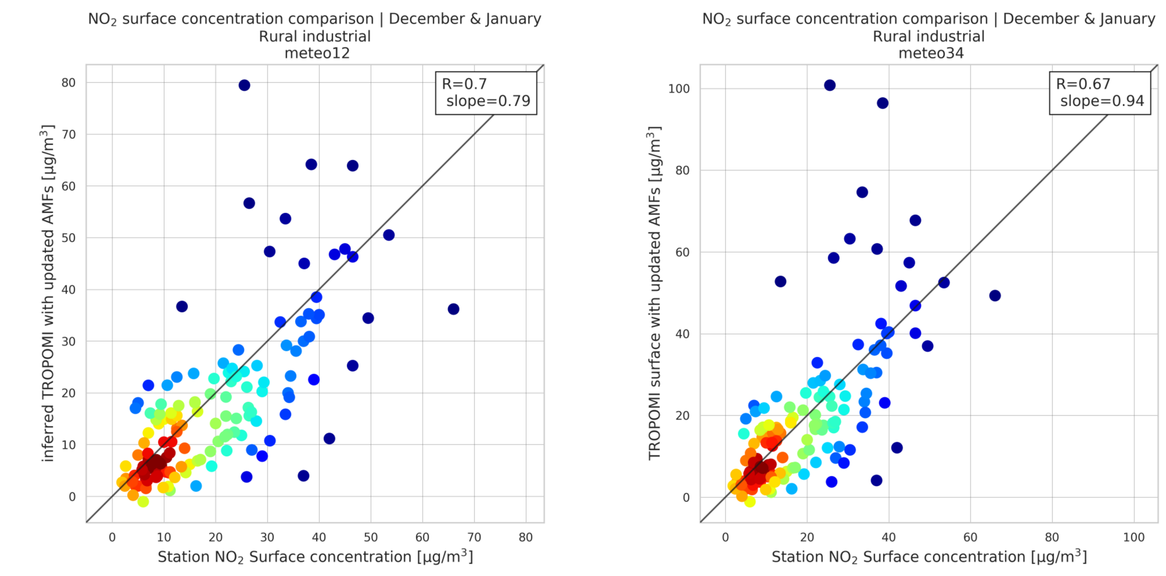

Figure 4. Scatter plots between the ground-based measurements and the inferred TROPOMI NO_2 surface concentrations of the rural industrial stations for the meteo12 [left] and the meteo34 [right] levelling schemes. The slope is closer to the unit in the case of the meteo34.

	Meteo12 levelling scheme			Meteo34 levelling scheme		
Station type	R	Slope	Relative bias (%)	R	Slope	Relative bias (%)
Urban traffic	0.47	0.81	-24.55	0.48	0.85	-20.70
Suburban traffic	0.43	0.65	-26.90	0.45	0.69	-23.18
Urban background	0.58	1.11	+7.40	0.58	1.13	**+12.00**
Suburban background	0.48	0.78	+3.90	0.49	0.86	**+10.90**
Rural background	0.53	0.67	+10.37	0.55	0.75	**+18.29**
Suburban Industrial	0.63	0.76	-15.66	0.62	0.82	-9.70
Rural industrial	0.7	0.79	-15.77	0.67	0.94	-4.32

Table 3. Statistics of the comparisons between the inferred and in-situ NO_2 surface concentrations for the two levelling schemes in winter. Meteo34 shows a better agreement with the ground-based measurements of the urban and industrial stations with improved statistical indicators. Both schemes overestimate the background concentrations, with the overestimations being higher in the meteo34 levelling scheme [red color]. Correlations are nearly identical for both schemes. Overall, meteo34 results in higher TROPOMI inferred NO_2 surface concentrations.

TROPOMI data version comparisons

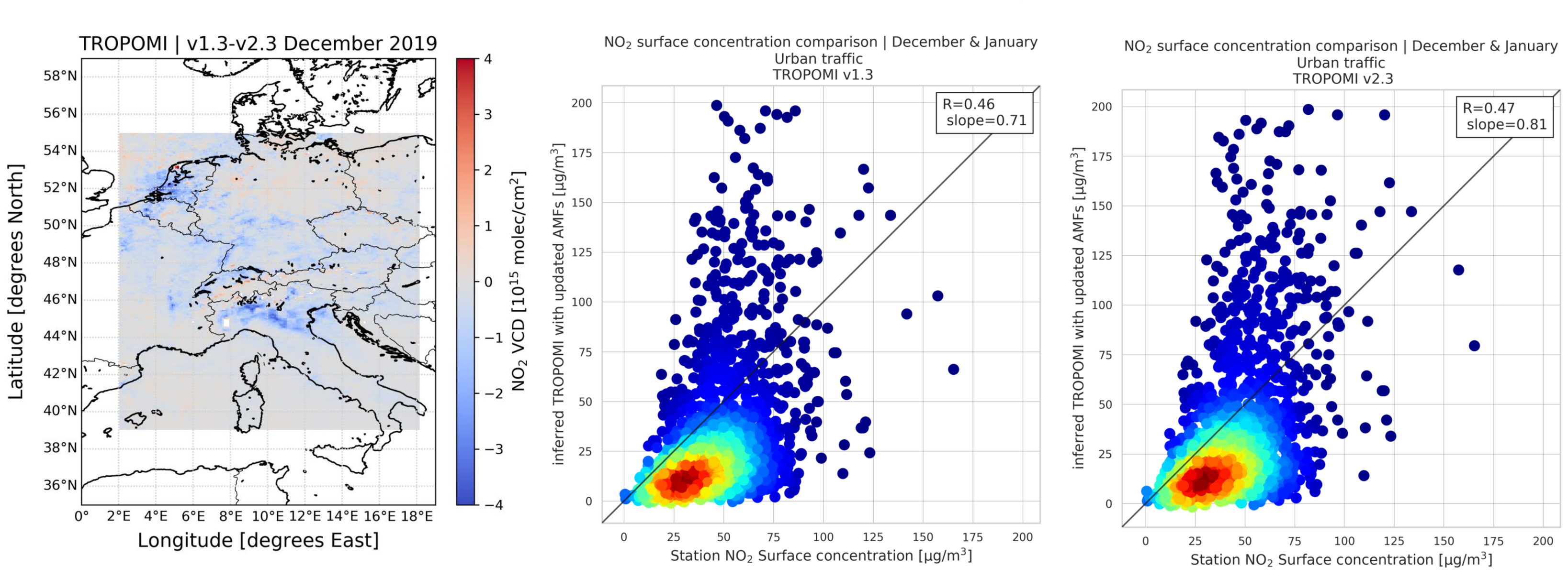

Figure 5. TROPOMI v1.3 and v2.3 TVCDs differences [left] and scatter plots between the ground–based measurements and the inferred TROPOMI v1.3 [middle] and v2.3 [right] NO_2 surface concentrations.

	TROPOMI v1.3		TROPOMI v2.3	
Station type	Absolute bias summer [μg/m³]	Absolute bias winter [μg/m³]	Absolute bias summer [μg/m³)	Absolute bias winter (μg/m³)
Urban traffic	29.45	15.46	28.00	10.46
Suburban traffic	25.88	20.19	24.75	11.53
Urban background	7.98	3.86	6.35	-2.21
Suburban background	4.82	2.27	3.27	-0.89
Rural background	3.47	**0.05**	3.17	-1.97
Suburban Industrial	7.76	7.46	6.11	3.77
Rural industrial	4.40	7.55	3.02	3.05

Table 4. Mean absolute bias [in μg/m³] between the in-situ and the inferred NO_2 surface concentrations for the two TROPOMI data versions for both periods. Traffic stations show the highest bias. Overall, TROPOMI v2.3 inferred data show lower biases for both periods, especially for the urban and suburban background stations. The bias for these stations is negative in winter, implying that an overestimation takes place. Also note that, v1.3 rural background stations bias is negligible in winter [blue color].

Application of the updated AMFs and AKs

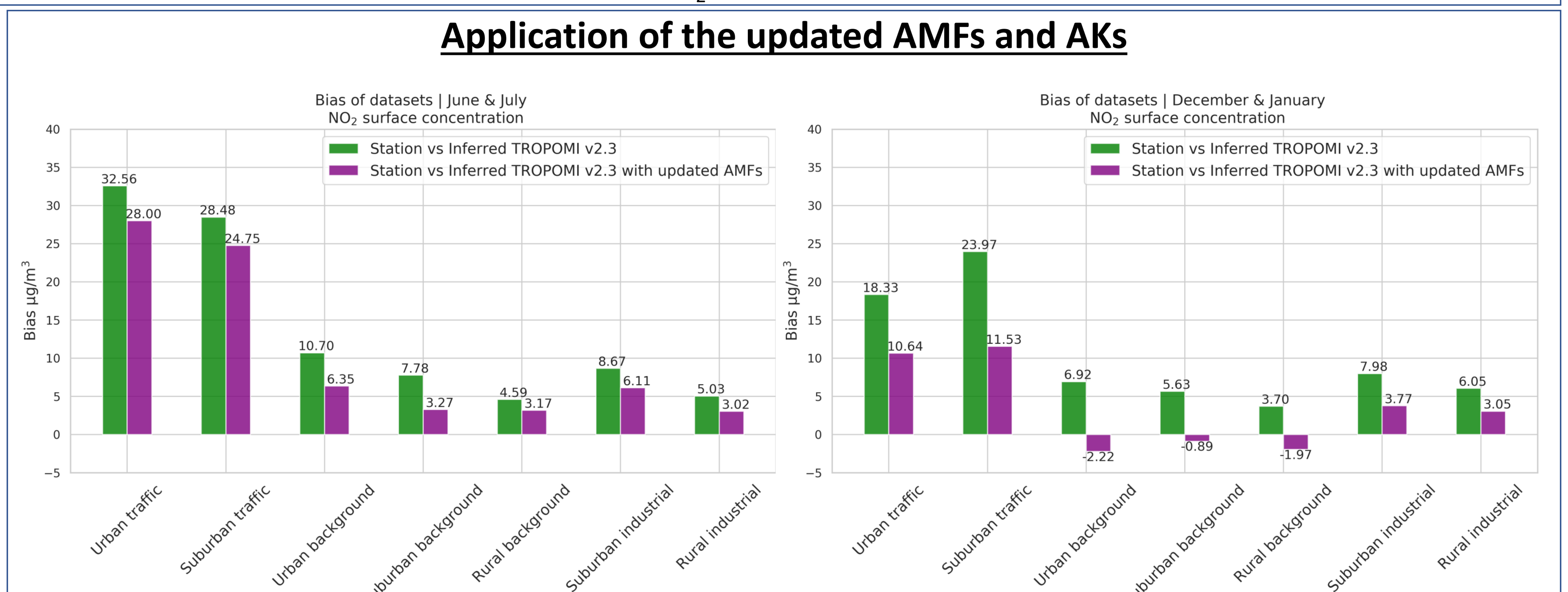

Figure 6. Mean absolute bias [in μg/m³] between the in-situ and the inferred NO_2 surface concentrations before the application of the updated AMFs [green] and after the application of the updated AMFs [purple]. For all station types and both periods, the updated datasets show lower biases. Background and industrial stations are closer to the ground-based truth.

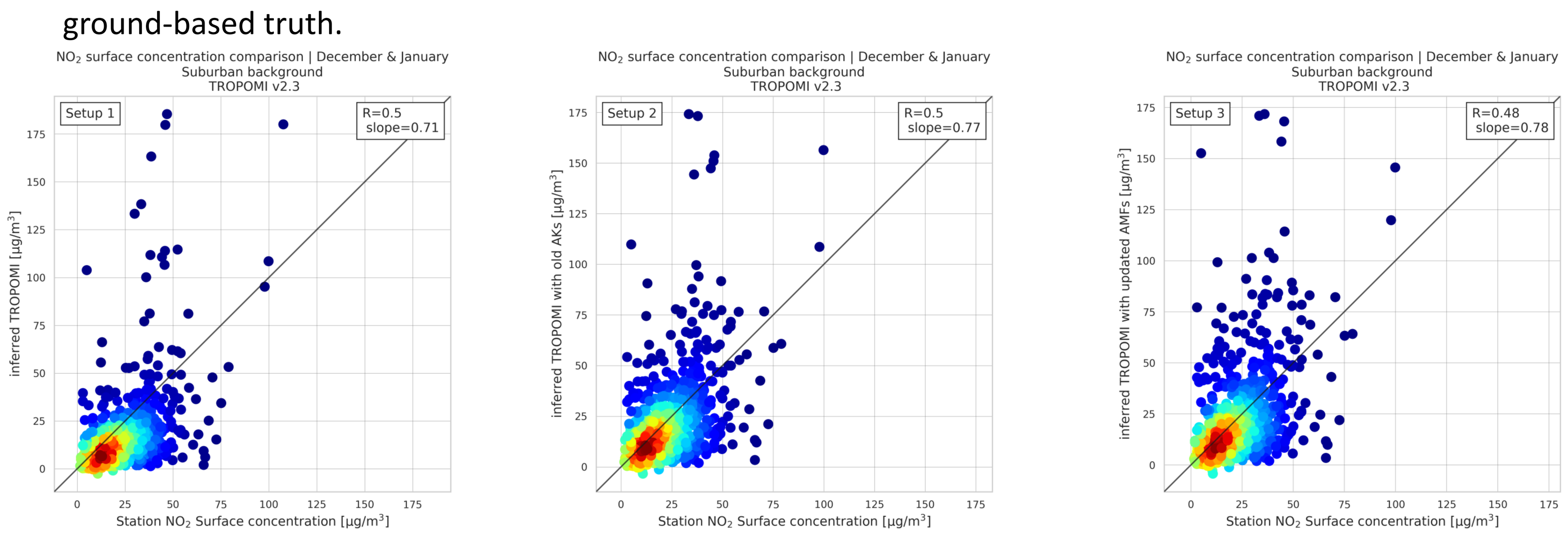

Figure 7. Scatter density plots of the suburban background stations with the in-situ measurements and the inferred TROPOMI v2.3 NO_2 surface concentrations for the 1st [left], 2nd [middle] and 3rd [left] setups.

Conclusions

- **TROPOMI v2.3 inferred NO_2 surface concentrations show reduced biases when compared to the v1.3 dataset. On an average and for all station types, bias is lower by 11% in summer and by 58% in winter.**
- **After the application of the updated AMFs and AKs on the satellite and model VCDs, the bias reduces by 24% in summer and by 67% in winter.**
- **The meteo34 NO_2 TROPOMI derived surface concentrations lie closer to the traffic and industrial ground-based measurements but overestimate the background stations measurements by approximately 6% when compared to the meteo12 dataset.**

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Data availability
- https://www.eea.europa.eu/data-and-maps
- https://data-portal.s5p-pal.com/
- https://lotos-euros.tno.nl/
- https://ci.tno.nl/gitlab/cams/cso

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Pseftogkas, A.; Koukouli, M.-E.; Segers, A.; Manders, A.; Geffen, J.v.; Balis, D.; Meleti, C.; Stavrakou, T.; Eskes, H. Comparison of S5P/TROPOMI Inferred NO_2 Surface Concentrations with In Situ Measurements over Central Europe. *Remote Sens.* **2022**, *14*, 4886. https://doi.org/10.3390/rs14194886