Validation of the ITMS TROPOMI NO_2 product

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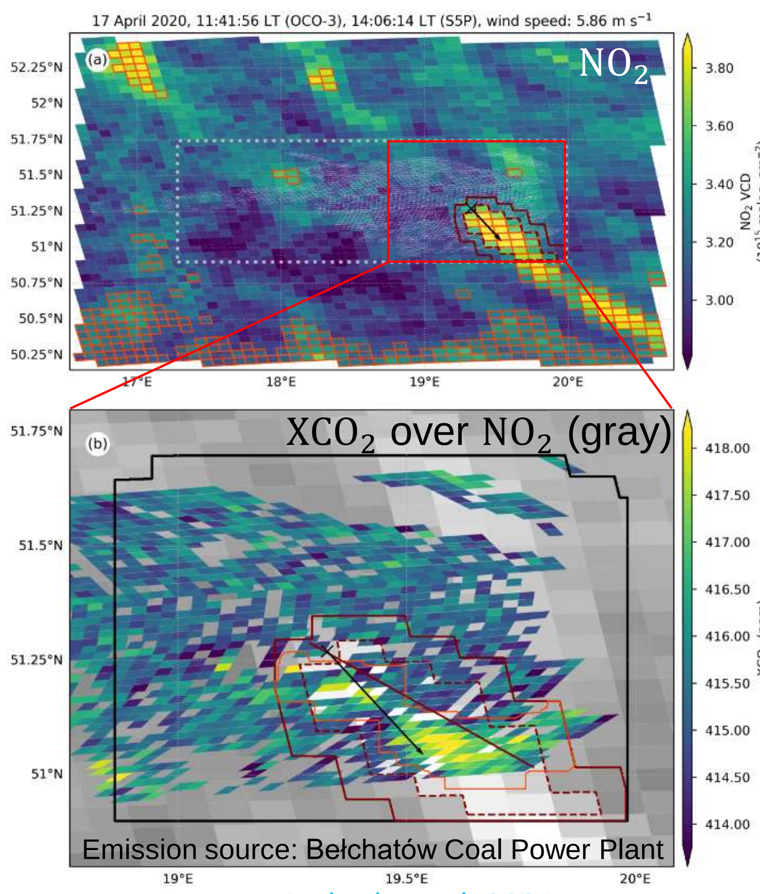
1. Motivation

CO_2 is the most important anthropogenic greenhouse gas. Detecting and quantifying CO_2 emission sources is an important task, but difficult to achieve, using satellite data. NO_2 is co-emitted with CO_2 during combustion processes and has short lifetime. Therefore, NO_2 plumes have a stronger gradient to surroundings, making NO_2 a useful proxy for CO_2 emissions.
The objective of this study is to establish a high resolution TROPOMI NO_2 product for Europe, optimised for small scale processes.



Fuentes Andrade et al. 2024

2. From spectrum to tropospheric vertical column

- Measure spectra using TROPOMI
- Fit spectra using DOAS method
  → total slant column (SC)
- Use STREAM to estimate strat. SC, subtract from total SC
  → tropospheric SC
- Transform into tropospheric VC using **A**ir **M**ass **F**actor (**AMF**)
- $AMF \stackrel{def}{=} \frac{SC}{VC}$, depends on a priori and surface reflectivity
- Use MODIS **Bi**-directional **R**eflectance **D**istribution **F**unction (**BRDF**) data for reflectivity (e.g. Zhou et al. 2010) to determine box-AMF (BAMF) using LUT
- Use CAMS-REG/CAMS global as NO_2 a priori to calculate AMF

$$AMF = \frac{\sum_i BAMF_i \cdot m_i \cdot c_i}{\sum_i m_i}$$

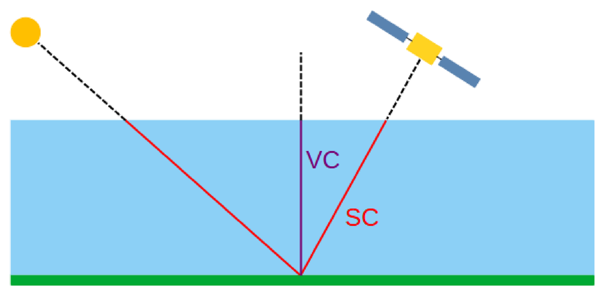
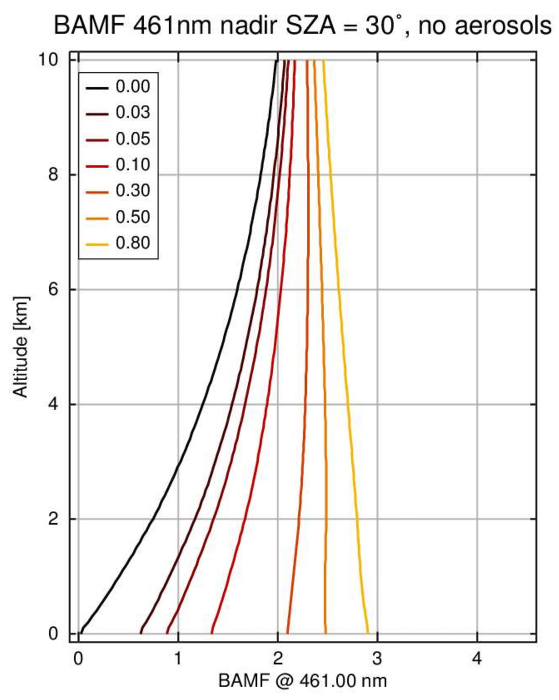
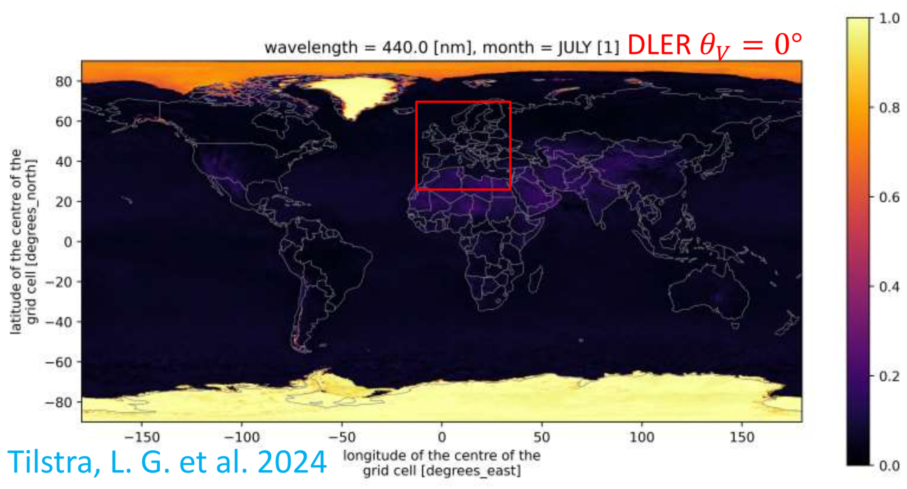


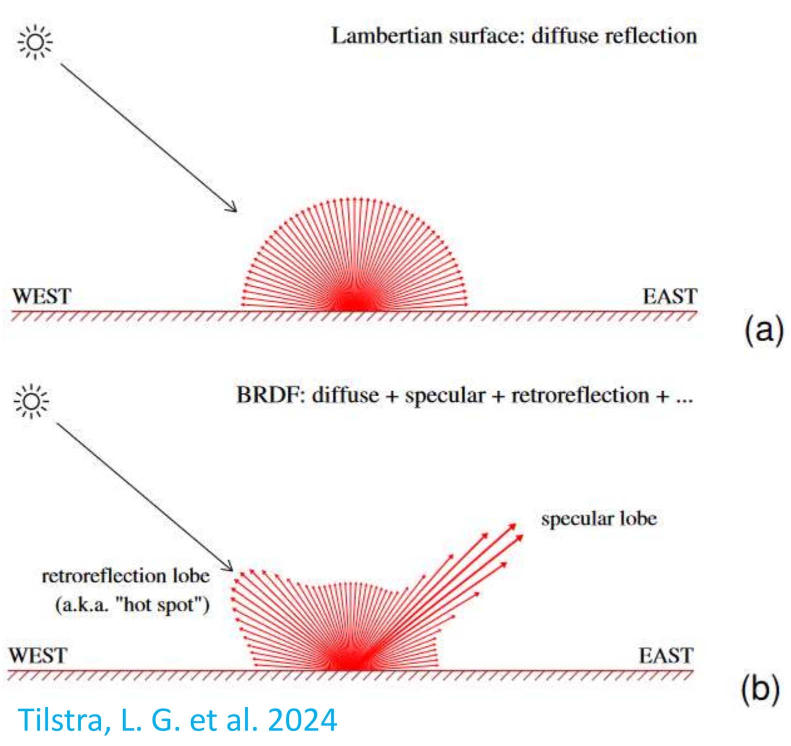
Illustration of slant and vertical columns.



Dependency of the Box AMF (BAMF) on the surface reflectivity. Small changes in reflectivity at low reflectivities lead to big changes in BAMF.



Tilstra, L. G. et al. 2024
Surface reflectivity of DLER product shows low reflectivities in target area (red)



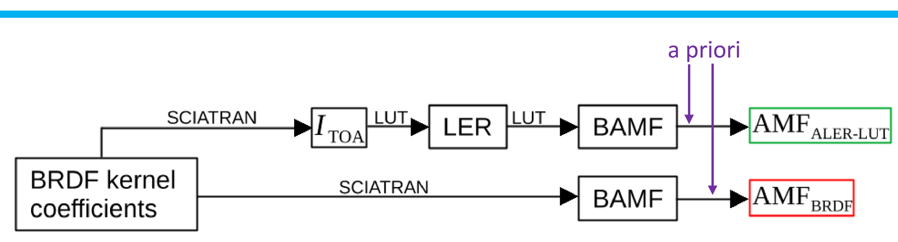
Tilstra, L. G. et al. 2024

a) Lambertian equivalent reflectivity (LER) reflected radiance in all directions the same

b) Bi-directional reflectance distribution function (BRDF), describes angle-dependent reflectivity of surfaces

3. AMF calculation

- AMF calculation using SCIATRAN and the BRDF for all TROPOMI pixels and orbits takes too long
- Shortcut: determine LER corresponding to TOA radiance of the BRDF case using LUT, as described by Vasilkov et al. (2017)



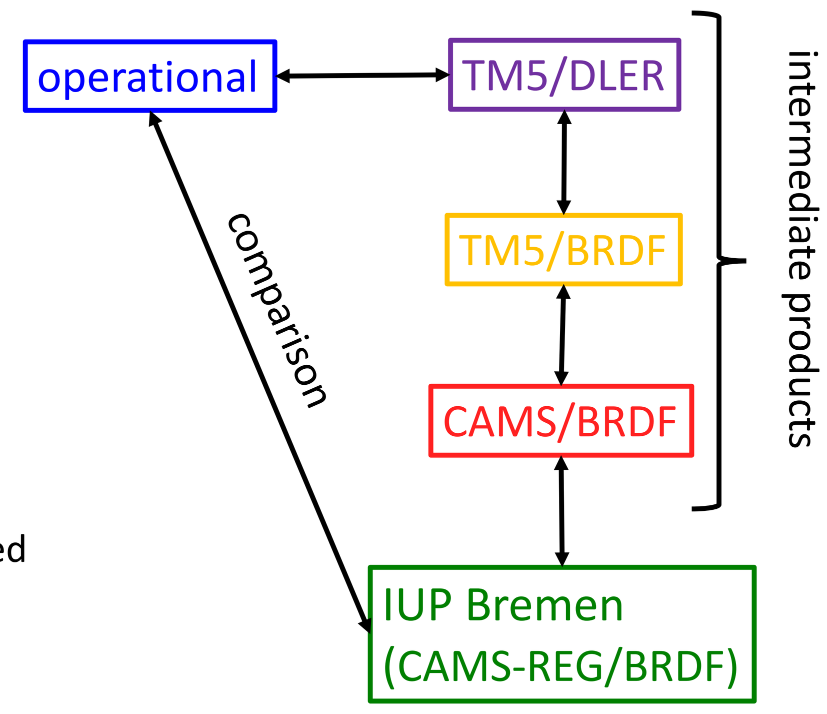
Flow chart for different AMF data sets

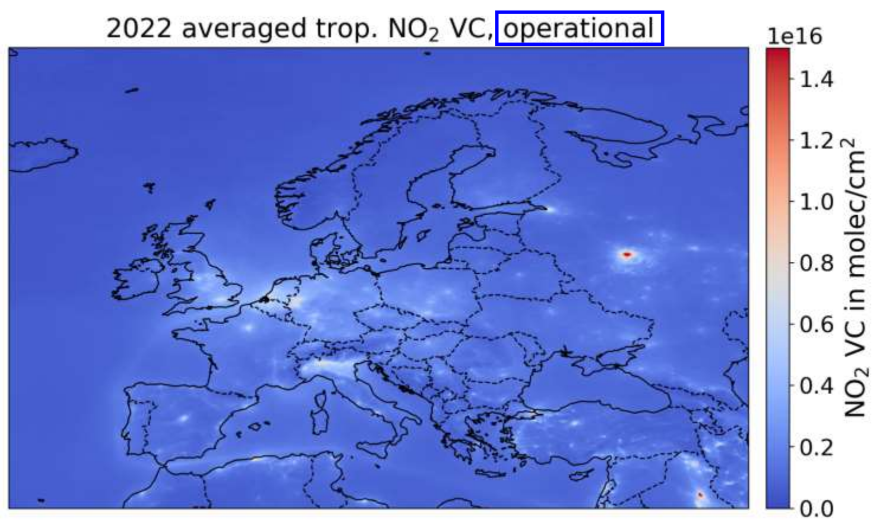
Legende
TOA… top of atmosphere
LUT… look-up table
ALER-LUT … angular LER-LUT

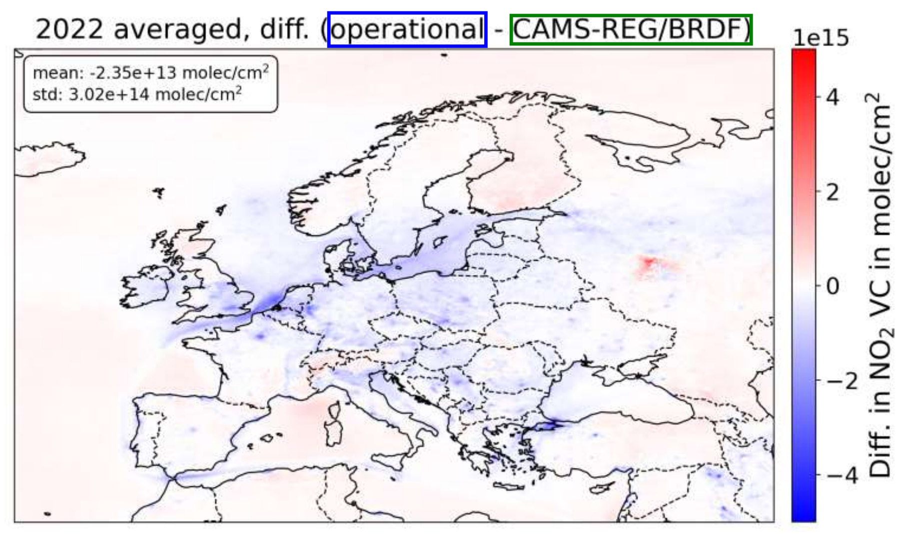
4. Results

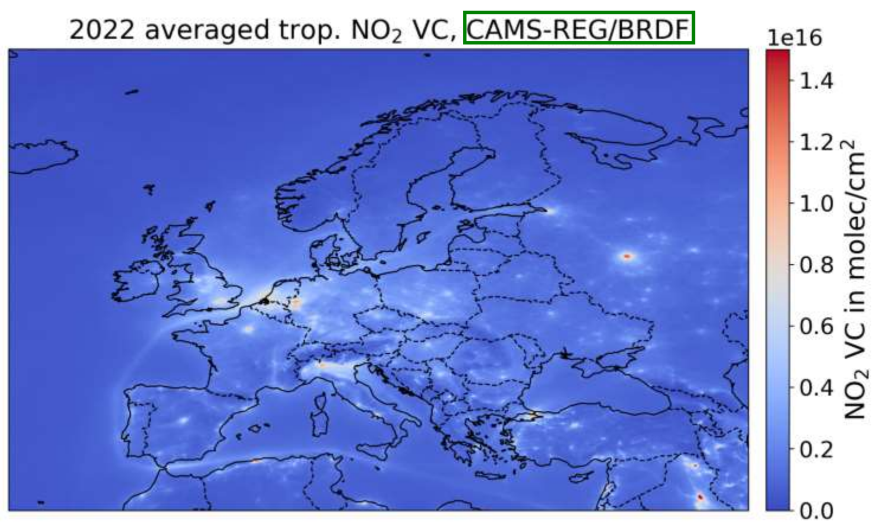
4.1 Sensitivity study

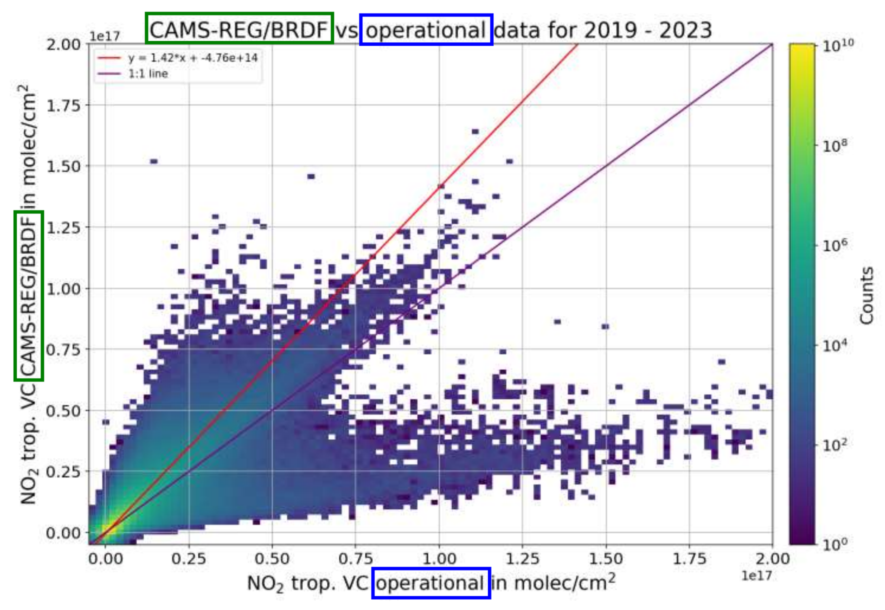
- IUP Bremen TROPOMI NO_2 product created, also called CAMS-REG/BRDF
- Multiple intermediate products created
- Differences operational and IUP Bremen product
  - Mostly due change of a priori
  - Influence of surface reflectivity smaller than expected
  - Most major hotspots and shipping lanes lower in operational product









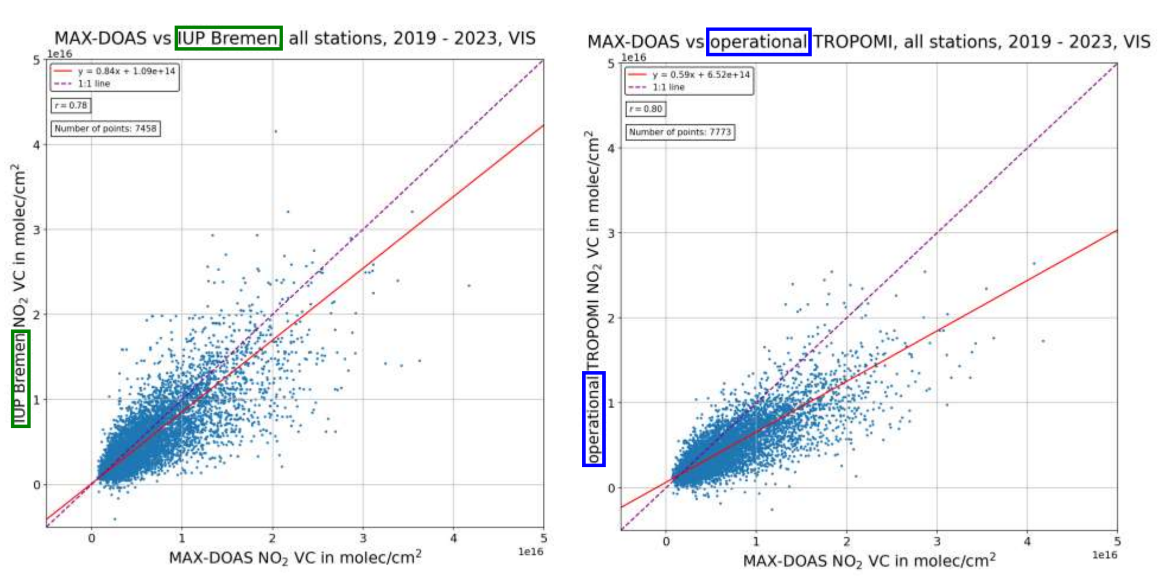


- Heat map of IUP Bremen vs operational product, IUP Bremen on average 42% larger
- Two additional branches found:
  - IUP Bremen > operational → mostly over water
  - IUP Bremen < operational → mostly over land

  Threshold of $\pm 2 \cdot 10^{16} \frac{molec}{cm^2}$ set, if difference larger (smaller) plot on map
- Number of affected points: $\sim 4.6 \cdot 10^5$, total points: $\sim 2 \cdot 10^{10}$ → rare outliers

4.2 Validation using MAX-DOAS data

- Average MAX-DOAS data for ±30 minutes around TROPOMI overpass
- Use TROPOMI pixel over MAX-DOAS sites, for IUP Bremen and operational data products
- IUP Bremen slightly lower correlation (0.78 to 0.8), but a slope closer to 1 (0.84 to 0.59)



Station by station statistics (VIS)

Product	IUP Bremen			operational		
Station	points	slope	corr.	points	slope	corr.
Athens	932	0.76	0.85	972	0.62	0.85
Bremen	792	0.83	0.74	830	0.61	0.75
Cabauw	787	0.91	0.80	598	0.60	0.80
De Bilt	722	0.95	0.78	755	0.65	0.78
Heidelberg	595	0.75	0.80	593	0.55	0.83
Mainz	1347	0.75	0.74	1253	0.54	0.80
San Pietro Capofiume	535	1.20	0.90	545	0.87	0.89
Thessaloniki	1494	0.85	0.77	1529	0.49	0.77
Uccle	274	1.02	0.69	298	0.64	0.75
all	7458	0.84	0.78	7773	0.59	0.80

- Slicing along years (not shown) reveals large difference in slopes and corr. from 2019 and 2021
- Data from 2021 and later show better statistics → Reason not yet known

5. Conclusions and outlook

- IUP Bremen TROPOMI NO_2 product created for 2019 – 2023
- Changing reflectance data base had lower impact on trop. VC than expected
- Changing a priori profile was more important
- IUP Bremen product larger than operational by 42%
- Comparison to MAX-DOAS shows improvement in slope, but slight decrease in correlation

- In the future: extending time series to 2024 (and later)
- Understand sudden improvement in statistics from 2019 to 2021

References
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