ASSESSMENT OF THE S-5P TROPOSPHERIC NO_2 PRODUCT BASED ON COINCIDENT AIRBORNE APEX OBSERVATIONS OVER POLLUTED REGIONS

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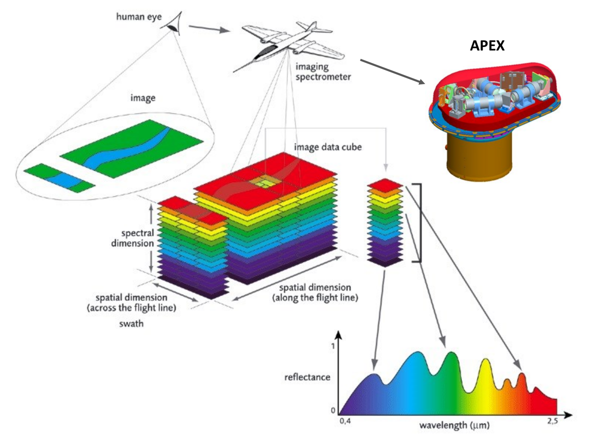
1 Introduction

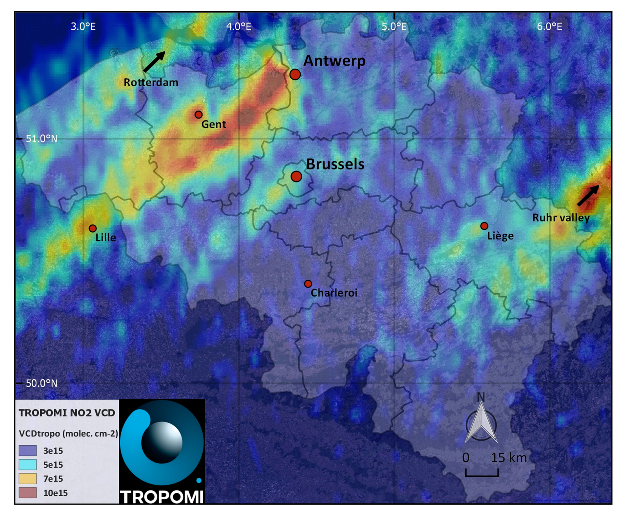
- Launched on 13 October 2017, **Sentinel 5 Precursor (S-5P)** is the first mission of the **EU Copernicus Programme** dedicated to the **monitoring of air quality, climate, ozone and UV radiation**.
- The **S-5P specs**, such as the much finer spatial resolution (3.5 by 5.5 km^2 at nadir), introduce many new opportunities and challenges, requiring **to carefully assess the quality and validity** of the generated data products by comparison with independent measurements.
- Airborne imagers such as **APEX** have demonstrated capabilities 1) to map the **horizontal distribution of pollutants like NO_2** at high resolution (~100 m^2) and with high accuracy, and 2) to provide reference data sets for **satellite validation**.



2 S5PVAL-BE campaign

- In the framework of the S5PVAL-BE campaign, the **S-5P/TROPOMI L2 tropospheric NO_2 product** has been validated over polluted urban regions based on comparison with coincident high-resolution APEX airborne remote sensing observations.
- **APEX has been deployed during 4 mapping flights** (26-29 June 2019) over the largest **urban regions in Belgium**, i.e. Brussels and Antwerp. In Antwerp, main NOx sources are related to (petro)chemical industry in the harbour, while traffic emissions are dominant in Brussels.

Right figure: Tropospheric NO_2 hotspots, observed over Belgium by TROPOMI (OFL v1.3) based on an early afternoon S-5P orbit on 27 June, 2019. Markers indicate the five largest Belgian cities. Long-range pollutant transport regularly occurs over Belgium, emitted from the strongly industrialised Rhine-Ruhr valley in Germany and the port of Rotterdam in The Netherlands.
Upper table: Mapping flight characteristics, and meteorological and environmental conditions for the four APEX flights.
Lower table: TROPOMI and APEX specifications for the S5PVAL-BE campaign, defined for APEX for a nominal altitude of 6.5 km a.g.l.

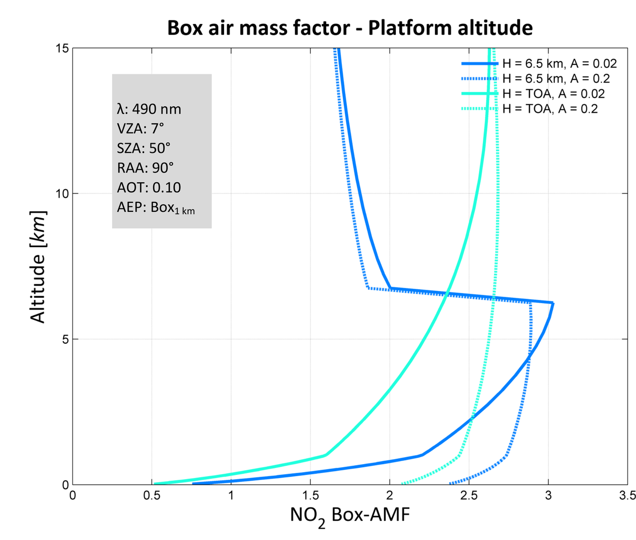


	Flight#1	Flight#2	Flight#3	Flight#4
Site	Brussels	Antwerp	Brussels	Antwerp
Date (day of year)	26-06-2019	27-06-2019	28-06-2019	29-06-2019
Flight time LT (UTC+2)	14:07–15:44	13:37–15:23	13:52–15:26	13:00–14:34
TROPOMI overpass LT (UTC+2)	13:16 (orbit 08811) 14:56 (orbit 08812)	14:37 (orbit 08826)	14:19 (orbit 08840)	14:00 (orbit 08854) 15:41 (orbit 08855)
# flight lines	12	11	12	11
Flight pattern	0°, 180°	0°, 180°	0°, 180°	0°, 180°
SZA	28°–36°	28°–34°	28°–34°	29°–30°
Average wind	4°	36°	49°	143°
Average wind speed	3.7 m s^{-1}	3.7 m s^{-1}	2.6 m s^{-1}	2.6 m s^{-1}
Average temperature	26° C	23° C	24° C	30° C
Average PBL height	684 m	888 m	798 m	No Data
Average AOT (440 nm)	0.57	0.16	0.15	0.09
Average AOT (500 nm)	0.51	0.15	0.15	0.10
Lat / Long	50.8° N / 4.4° E	51.2° N / 4.4° E	50.8° N / 4.4° E	51.2° N / 4.4° E
Average terrain	76 m	10 m	76 m	10 m

	TROPOMI (UVIS)	APEX (VNIR)
Orbit	Polar, sun-synchronous	-
Temporal resolution	Daily global coverage (13:30 local solar time)	-
Wavelength range	305–499 nm	370–970 nm
Spectral resolution (FWHM)	0.45–0.65 nm	1.5–3.0 nm
FOV across-track	108°	28°
IFOV across track	0.24°	0.028°
Flight altitude	824 km	6.5 km
Swath width	2600 km	3.2 km
Ground speed	7800 m s^{-1}	72 m s^{-1}
Across-track spatial resolution (nadir)	3500 m	60 m
Along-track spatial resolution (nadir)	7000 m[a]	80 m
Signal-to-noise	800-1000	2500
NO_2 VCD detection limit (molec cm^{-2})	~1.4×10^{15}	~2.2×10^{15}
Temperature stabilisation	Yes	Yes
Radiometric calibration	Yes	Yes
Weight	220 kg	354 kg
Size (LxWxH)	0.75x0.56x1.4 m^3	0.83x0.64x0.56 m^3
Power consumption	170 W	2100 W
Scanning	Pushbroom	Pushbroom

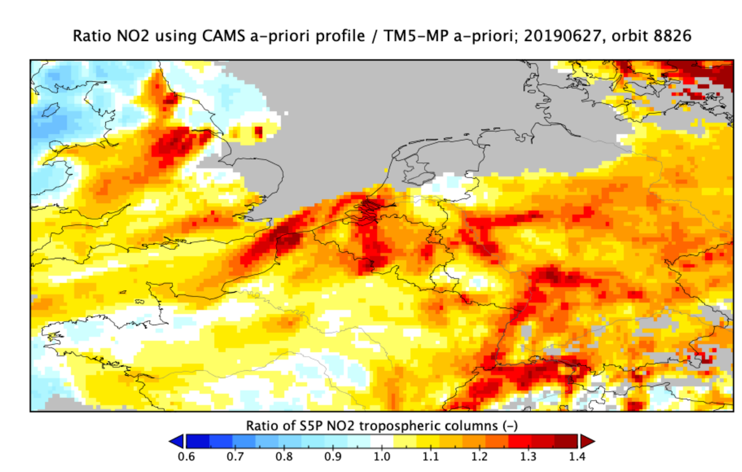
3 NO_2 VCD retrieval algorithm

- The TROPOMI (van Geffen et al., 2018) and APEX (Tack et al., 2017) NO_2 vertical column density (VCD) retrieval schemes are similar in concept and based on
  - 1) **Differential Optical Absorption Spectroscopy (DOAS)** fitting of the pre-processed spectra in the visible wavelength region.
  - 2) **Calculation of appropriate air mass factors (AMFs)** by a radiative transfer model in order to account for enhancements in the optical path length due to the surface albedo, aerosol and NO_2 profile shapes and viewing and sun geometry.
  - 3) Finally, retrieved L2 NO_2 VCDs are **georeferenced, gridded and intercompared** by averaging the coincident APEX VCDs within the TROPOMI pixels. Per flight, ~10 to 20 TROPOMI pixels were fully covered by APEX pixels with an absolute time offset of smaller than 1 hour. Depending on the TROPOMI pixel size, each pixel consists of ~2400 to 4000 APEX pixels.



Height-dependent box-AMFs assess the instrument's vertical sensitivity to NO_2, illustrated for both the aircraft and TROPOMI altitude, for both low and high surface reflectance scenarios. The instrument is the most sensitive to the layer directly under the sensor. Due to scattering and absorption, the sensitivity decreases towards the ground surface. The decrease in sensitivity is stronger with increasing platform altitude.

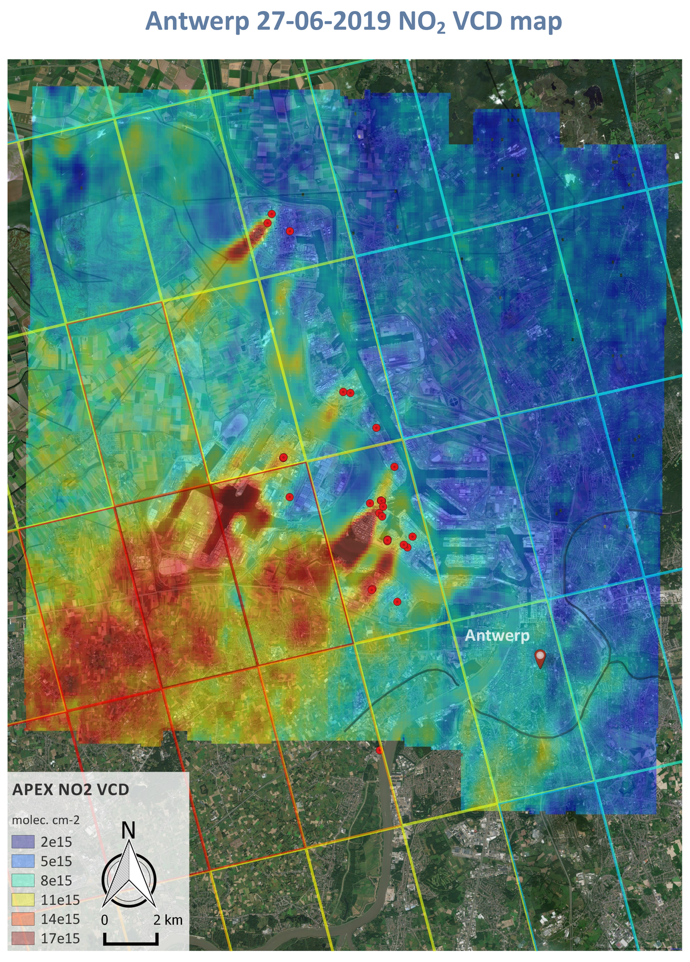
- To better resolve sharp gradients in strongly polluted areas, comparisons are done as well with a custom TROPOMI tropospheric NO_2 product, calculated based on **NO_2 profile shapes from the Copernicus atmospheric monitoring service (CAMS) regional ENSEMBLE (0.1°)** instead of TM5-MP a-priori NO_2 profiles (0.5°).



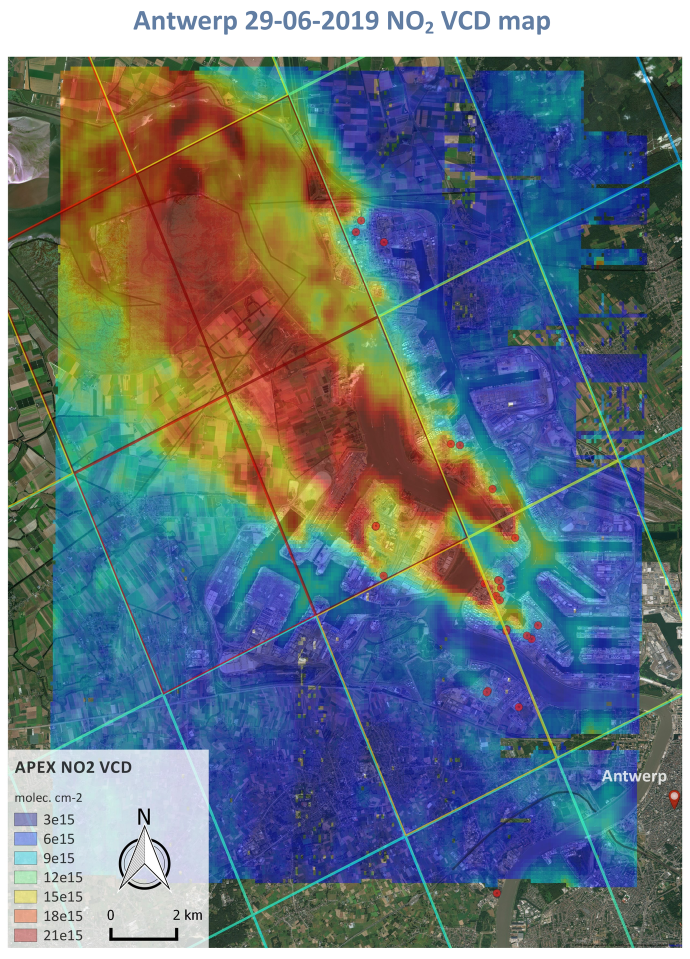
- The overall errors in the tropospheric NO_2 columns are fully characterized in van Geffen et al. (2018) and Tack et al. (2017) for TROPOMI and APEX, respectively. The accuracy of the TROPOMI tropospheric NO_2 product is expected to be around **25-50% with a precision of 0.7 x 10^{15} molec cm^{-2}** (Fehr, 2016). The APEX relative VCD error is around **20 -35%** at its native spatial resolution and is expected to be further improved by spatial averaging within the TROPOMI pixel.

4 Results

Antwerp 27-06-2019 NO_2 VCD map



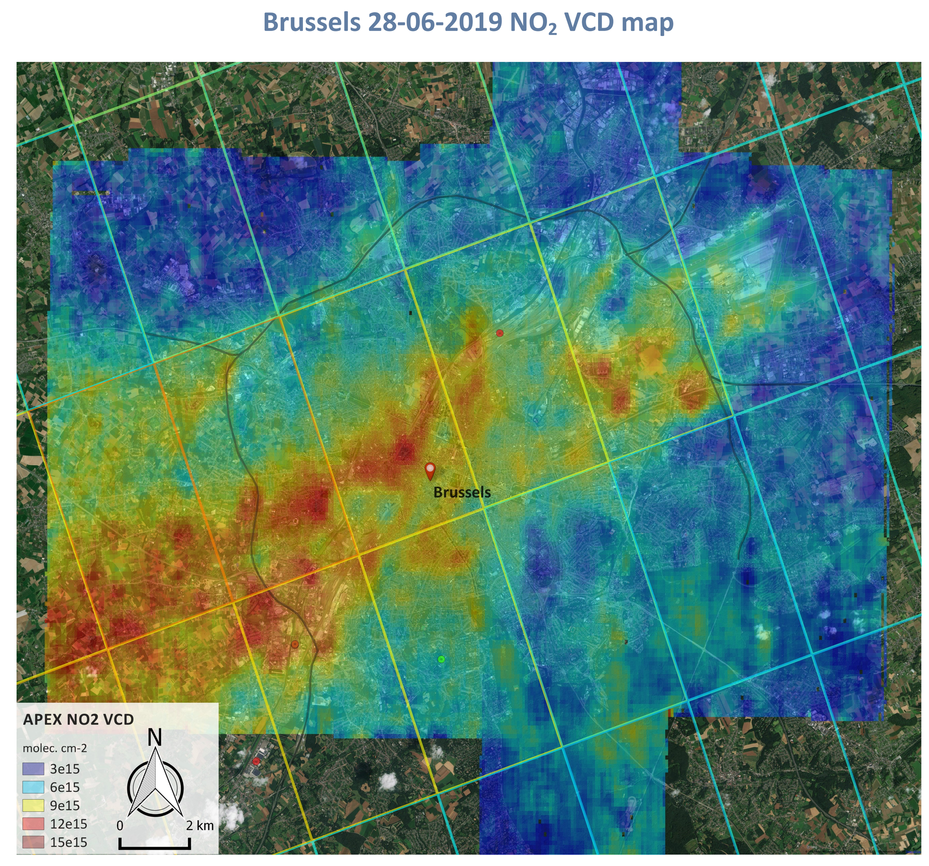
Antwerp 29-06-2019 NO_2 VCD map



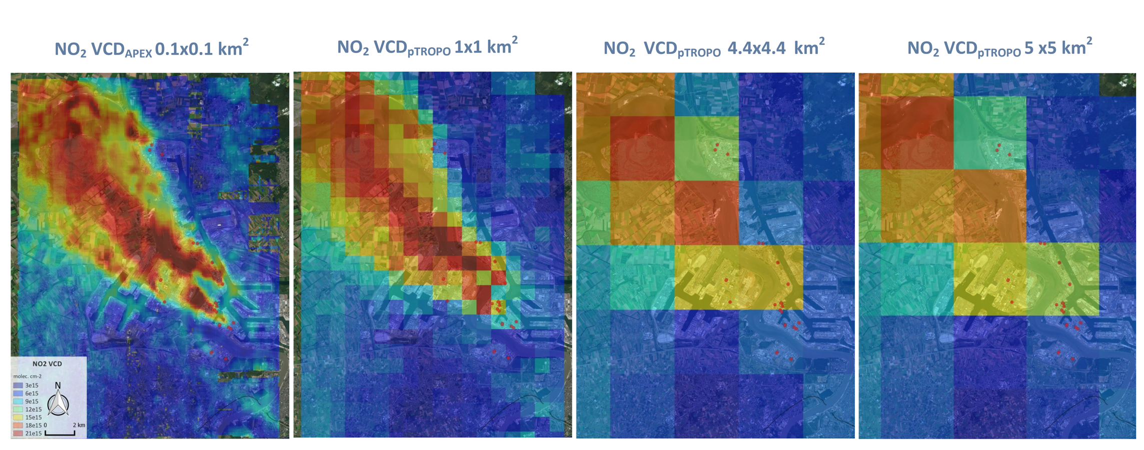
Upper panels: Retrieved APEX NO_2 VCD maps are shown for June 27-29, 2019. The data was acquired in cloud-free conditions with a low AOD (<= 0.10). Red dots indicate point sources from the emission inventory (2017), emitting more than 10 kg of NOx per hour. Key highways and ring roads are indicated by black lines. TROPOMI retrievals are overlayed as color-coded polygons.

The maps reveal that the NO_2 field can be highly variable in urban areas both in space and time. The NO_2 levels observed by APEX range between 1 and 40 x 10^{15}, and 1 and 24 x 10^{15} molec cm^{-2} in Antwerp (mainly industrial emissions) and in Brussels (mainly traffic emissions), respectively. Strong patterns of enhanced NO_2 can be discerned: some detailed confined plumes can be linked to individual stacks, while clusters of stacks contribute together to larger plumes. Also increased values can be observed along the ring roads and junctions with the key highways. The observed plumes are narrow and confined close to its sources and transported downwind for several tens of kilometers. TROPOMI retrievals exhibit in general a good consistency with the APEX retrievals. However, elevated levels of NO_2 from isolated hotspots and narrow and confined plumes, visible in the APEX retrievals, cannot be spatially resolved anymore by TROPOMI and are averaged out within the TROPOMI pixel.

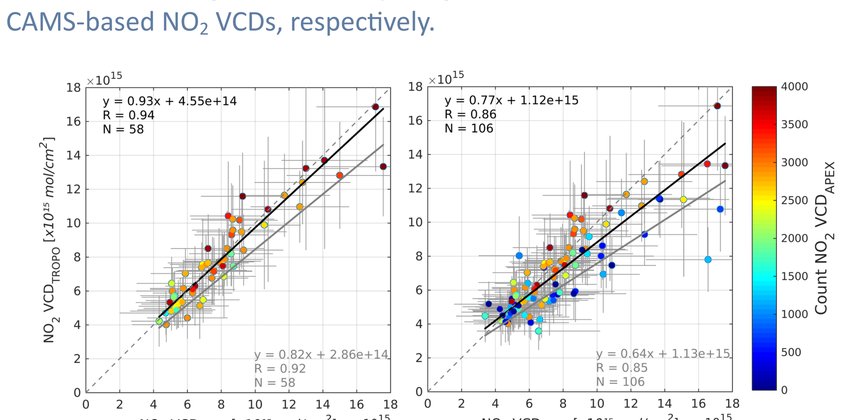
Brussels 28-06-2019 NO_2 VCD map

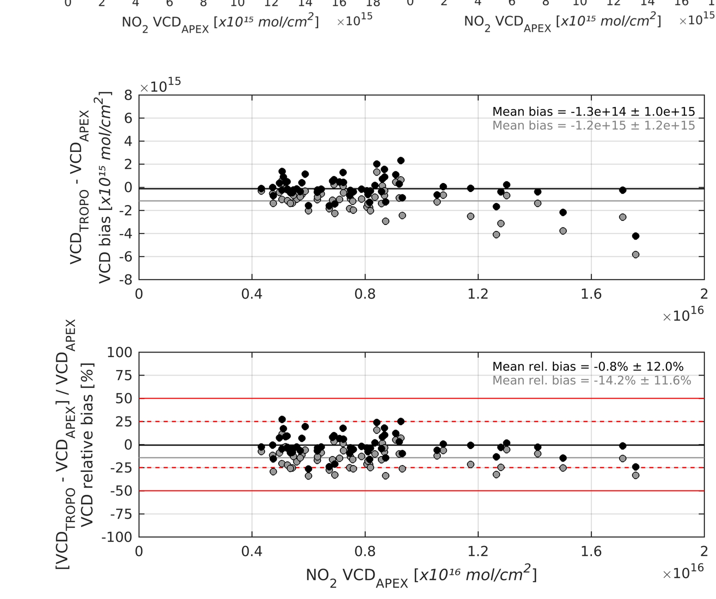


Lower panel: (a) APEX NO_2 VCD grid retrieved over Antwerp on 29 June, at 100 m resolution, and regridded to pseudo-satellite NO_2 VCDs grids at (b) 1 x 1 km^2, (c) 4.4 x 4.4 km^2, and (d) 5 x 5 km^2, respectively. At the resolution of 1 km, different plumes can still be resolved and they can be largely linked to the key emission sources, such as the stacks in the harbour and the Antwerp ring road. However, at the resolution of 4.4 and 5 km^2 the signal is smoothed and only one merged plume can be distinguished downwind while it is not trivial to pinpoint its source(s). The amount of underestimation of peak plume values and overestimation of urban background values in the TROPOMI data is in the order of 1-2 x 10^{15} molec cm^{-2} on average, or 10% - 20%, depending on the amount of heterogeneity in the NO_2 field and assuming a TROPOMI pixel size of 3.5 x 7 km^2.



Lower panels: Scatterplot and orthogonal linear regression analysis of co-located TROPOMI and averaged APEX NO_2 VCD retrievals for the four flights. Regression lines and statistics are color-coded black and grey for the comparison of APEX NO_2 VCDs with CAMS-based TROPOMI NO_2 VCDs and TM5-MP-based VCDs, respectively. Vertical error bars indicate the overall error in NO_2 VCD_{TROPO}, while the horizontal whiskers represent the error in NO_2 VCD_{APEX} retrievals, averaged over all APEX pixels within the boundaries of a co-located TROPOMI pixel. Data points are color-coded based on the number of APEX pixels averaged within a TROPOMI pixel. **Left figure** only shows the comparison when a TROPOMI pixel is at least covered half by APEX pixels while the **right figure** shows the comparison for all TROPOMI pixels having coincident APEX pixels. The larger bias due to undersampling can be observed. Overall for the ensemble of the four flights, the standard TROPOMI NO_2 VCD product is well correlated (R = 0.92) but biased negatively by -1.2 ± 1.2 x 10^{15} molec cm^{-2} or -14% ± 12%, on average, with respect to coincident APEX NO_2 retrievals. When replacing the coarse 1° x 1° TM5-MP a priori NO_2 profiles by NO_2 profile shapes from the CAMS regional CTM ensemble at 0.1° x 0.1°, the slope increases by 11% to 0.93, and the bias is reduced to -0.1 ± 1.0 x 10^{15} molec cm^{-2} or -1.0% ± 12%. When the absolute value of the difference is taken, the bias is 1.3 x 10^{15} molec cm^{-2} or 16%, and 0.7 x 10^{15} molec cm^{-2} or 9% on average, when comparing APEX NO_2 VCDs with TM5-MP-based and CAMS-based NO_2 VCDs, respectively.





5 Summary and Perspectives

- **Independent validation** of the end-to-end mission performance is essential for the determination of the S-5P data quality. L2 TROPOMI NO_2 VCDs are **well correlated (R > 0.9) but biased low** with respect to airborne APEX NO_2 retrievals. The bias is smaller when compared to the custom product, based on CAMS regional ENSEMBLE as it better captures the strong gradients in urbanised areas. However, both the standard and custom product are within the targeted bias of 25-50% for the tropospheric NO_2 product.
- The APEX data set allows as well to study the **TROPOMI subpixel variability and impact of signal smoothing** due to its finite satellite pixel size, typically coarser than fine-scale gradients in the urban NO_2 field. The amount of underestimation of peak plume values and overestimation of urban background values in the TROPOMI data is in the order of 1-2 x 10^{15} molec cm^{-2} on average, or 10% - 20%, depending on the amount of heterogeneity in the NO_2 field and assuming a TROPOMI pixel size of 3.5 x 7 km^2.
- The NO_2 standard product could be further improved for retrievals over polluted regions by making use of 1) **a priori NO_2 profiles from a high-resolution CTM**, such as the CAMS-regional ensemble at 0.1° and 2) an **albedo product at higher resolution** than the OMI LER in order to resolve the strong albedo variability.
- The applied **validation strategy for TROPOMI tropospheric NO_2 retrievals** based on airborne mapping data can be valuable for validation of future satellite missions, such as S-5, S-4, TEMPO and GEMS.

6 References and Acknowledgements

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- S-5P is a European Space Agency (ESA) mission implemented on behalf of the European Commission (EC). The TROPOMI payload is a joint development by ESA and the Netherlands Space Office (NSO).
- The S5-p results shown in this presentation contain modified Copernicus Sentinel data, processed by BIRA-IASB/DLR/KNMI/ESA.
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