S5P MPC VDAF Validation Web Article: Nitrogen Dioxide Column Data

Contributing authors

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Product definition

The following table contains a description of the S5P TROPOMI processor versions evaluated in this report.

Processor Version	In operation from	In operation until
01.00.01*	RPRO: orbit 01575 (Feb 1st 2018)	RPRO: orbit 02880 (May 4th 2018)**
01.00.02	NRTI: orbit 03365 (June 7th 2018)	NRTI: orbit 03943 (July 18th 2018)**

* The RPRO NO_2 dataset was reprocessed in offline mode using Level 1 version 01.01.00 data.

** The validation analysis reported hereafter was carried out on RPRO data up to orbit 02398 (March 31th 2018), and on NRTI data up to orbit 3400 (June 9th 2018).

The RPRO data evaluated in this report was generated with the OFFL processor. This data set was available to the S5P Mission Performance Centre (MPC) and the S5P AO Validation Team (S5PVT) for validation purposes only, and not distributed publicly. Currently, public access to OFFL-processed data is grated for data sets with measurement date starting on June 28th 2018 (DOI: http://doi.org/10.5270/S5P-s4ljg54).

Product requirements are described in the Sentinel-5 Precursor Calibration and Validation Plan for the Operational Phase source: ESA; ref: ESA-EOPG-CSCOP-PL-0073; issue: 1.0 date 2017-06-11, Sentinel-5P-Calibration-and-Validation-Plan.pdf.

Initial validation results

This report describes initial validation results for Sentinel-5p TROPOMI L2_NO_2 tropospheric column, stratospheric column and total column data: tropospheric and total NO_2 column data retrieved with the OFFL processor (v1.0.1), and stratospheric column data retrieved with the OFFL processor (v1.0.1) and the NRTI processor (v1.0.2).

The validation analyses summarised in this article were carried out in May and June 2018 and reported at the 1st Product Release Workshop held at ESA/ESRIN on June 25-26, 2018 (https://nikal.eventsair.com/QuickEventWebsitePortal/sentinel-5p-first-product-release-workshop/sentinel-5p).

Stratospheric NO_2 column

Comparison with NDACC UV-Vis ZSL-DOAS data

TROPOMI L2_NO_2 stratospheric column data have been compared to UV-Vis zenith-scattered-light twilight DOAS (ZSL-DOAS) measurements collected from the Network for the Detection of Atmospheric Composition Change (NDACC). Both the S5P MPC Validation Data Analysis Facility (VDAF) and the Multi-TASTE expert validation system have been used for data handling, harmonisation and comparison.

The majority of the UV-Vis validation data have been obtained through the SAOZ real time processing facility operated by the CNRS LATMOS (Laboratoire Atmosphères, Milieux, Observations Spatiales). All those preliminary data have been quality-controlled by BIRA-IASB's Multi-TASTE/CORR_2 system. Only TROPOMI pixels with `qa_value` > 0.5 have been considered, in accordance with recommendations expressed in the Product Readme File. Note that this includes cloud-covered pixels; for tropospheric NO_2 one could expect smaller discrepancies with the stricter filter `qa_value` > 0.75, but for stratospheric NO_2 the effect should not be significant. To reduce mismatch errors due to the significant difference in horizontal smoothing between TROPOMI and ground-based measurements, TROPOMI ground pixels (at high horizontal resolution) have been averaged over the polygon representing the airmass measured by the UV-Vis zenith-scattered-light spectrometers (see left-hand panel in Figure 1).

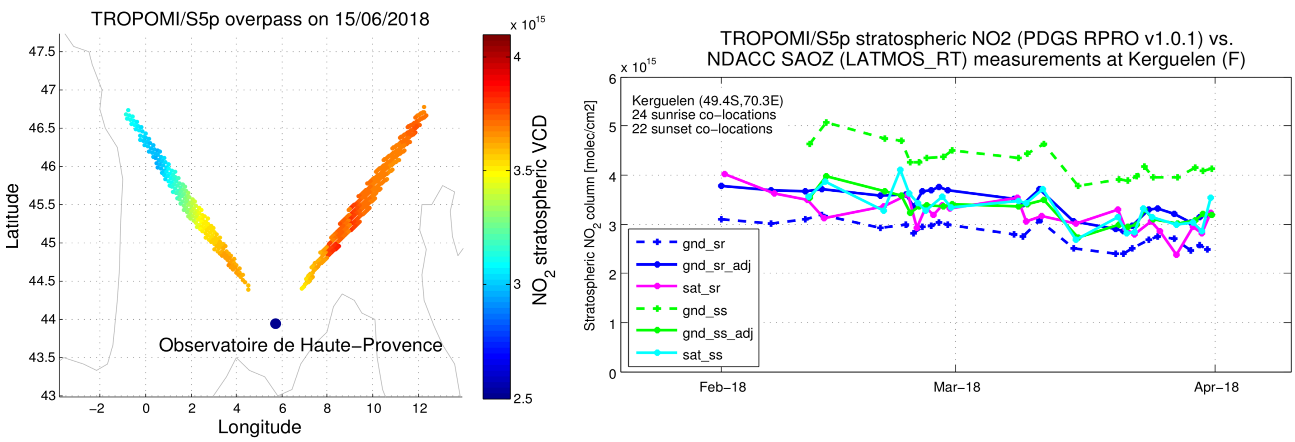

Figure 1: Left: illustration of the averaging of TROPOMI ground pixel values over the actual area of sensitivity of a ZSL-DOAS ground-based measurement. Right: illustration of the effect of the photochemical time correction between sunrise or sunset and the TROPOMI solar local time.

Over the period tested (February up to end of March 2018) and with respect to the validation data available at the time of this analysis, roughly 40 co-locations at 10 NDACC UV-Vis/SAOZ stations have been identified, sampling latitudes regularly from the Arctic to the Antarctic. Due to the large temporal difference between the satellite (S5P solar local time at ascending node at ~13:30) and validation measurements (at sunrise and sunset), a model-based photochemical time adjustment has been applied to account for the diurnal cycle of stratospheric NO_2 (see right-hand panel of Figure 1 for an illustration). Twilight reference data were adjusted to the solar local time at the TROPOMI ground pixel centre.

The mean and standard deviation of the difference are shown, per station and as a function of latitude, in Figure 2. From these comparisons, the following conclusions can be drawn:

- Both the mean difference (bias) and comparison spread (1 sigma) range within the mission requirements: at most 10% bias and 0.5 Pmolec/cm^2 uncertainty.
- The level of agreement is similar to the one reported with preceding UV-Vis nadir sounders such as Envisat SCIAMACHY and GOME-2A.
- TROPOMI underestimates ground-based values of the stratospheric column by about 0.2 ± 0.3 Pmolec/cm^2. The range refers to the station-to-station scatter and not the uncertainty on the mean.
- First analyses reveal no obvious influence of solar zenith angle and cloud fraction on the comparison results. Based on a limited set of orbits, this preliminary conclusion needs to be confirmed.

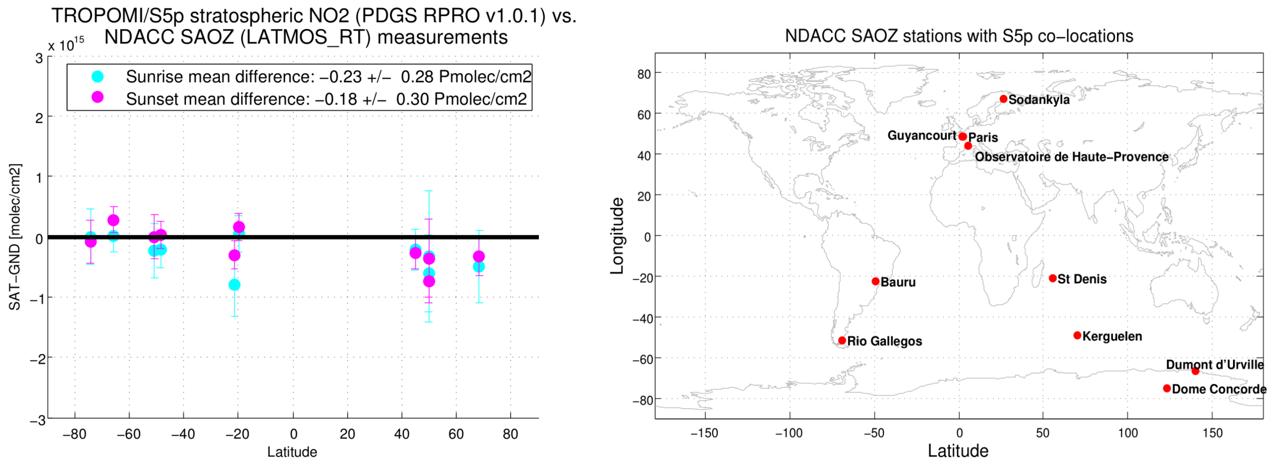

Figure 2: Left: latitude distribution of the mean difference (circular marker) and of the standard deviation of the difference (error bar) between TROPOMI and NDACC ZSL-DOAS data, at the 10 SAOZ stations identified in the right panel. Note that this graph includes only RPRO (OFFL processor) data; however, initial validation results indicate that the NRTI data perform similarly. The error bar reported in the legend corresponds to the station-to-station scatter, not to the uncertainty on the mean difference (bias).

Tropospheric NO_2 column

Comparison with NDACC UV-Vis MAX-DOAS data

TROPOMI L2_NO_2 tropospheric column data has been compared to NDACC UV-Vis Multi-Axis DOAS (MAXDOAS) measurements processed in Rapid-Delivery mode. Only TROPOMI ground pixels associated with a quality value (`qa_value`) > 0.75 have been selected, in accordance with recommendations expressed in the Product Readme File. Over the period tested (February up to end March 2018) and with respect to the validation data available at the time of this analysis, 3 sites contributed to the comparison, with 3 (De Bilt) up to ~12 (Cabauw, Xianghe) co-locations identified per site. Only TROPOMI ground pixels containing the MAXDOAS instrument site were considered. Per satellite overpass, the average is taken of all MAXDOAS measurements in a 2h time interval centered at the satellite measurement time.

Results:

- A negative bias is detected for the three sites, which is within the product requirement of 50% (Figure 3).
- The spread of the difference between TROPOMI and MAX-DOAS data is larger than the precision requirement of 0.7 Pmolec cm^{-2}, but there is likely a large contribution of validation measurement and comparison errors to the spread (Figure 3).

- Influence quantities: the potential influence of several quantities has been investigated (solar zenith angle, viewing zenith angle, aerosol index, cloud properties etc.) but no firm conclusions can be drawn from the small data sample. A larger negative difference with increasing AMF might be expected (Figure 4).
- Comparing the cloud pressure (CP) values available in the S5P NO_2 product file with the cloud pressure value of the S5P CLOUD CRB product reveals a possible issue: several pixels with CP predicted to be ~1 bar by S5P NO_2, are considerably lower in CP according to S5P CLOUD CRB (Figure 4). Note that in Figure 4, a `qa_value` > 0.5 instead of > 0.75 is taken, such that cloudy situations are included as well.

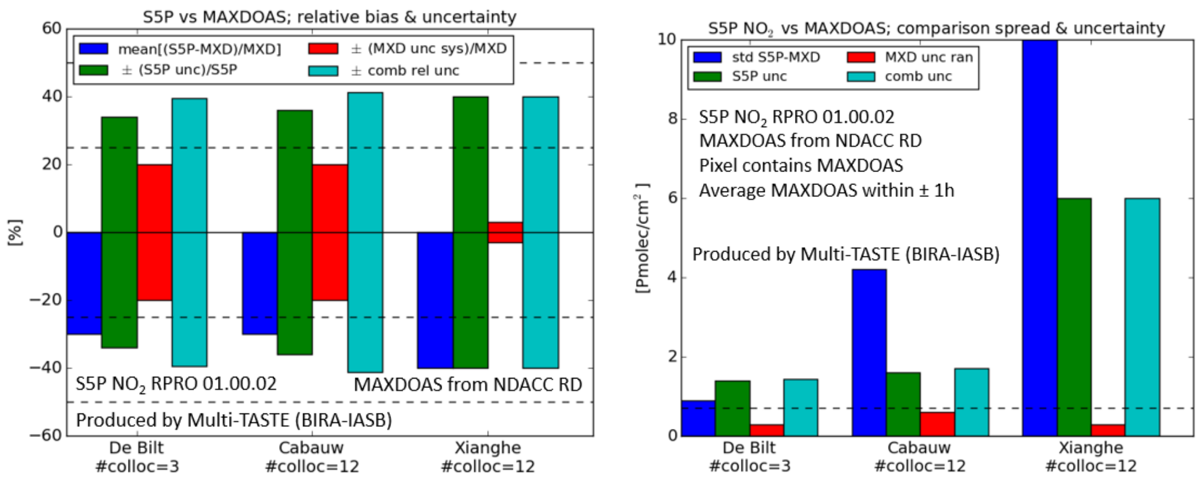

Figure 3. Left: mean relative difference between S5P and MAXDOAS tropospheric NO2 column values (blue), ex-ante relative uncertainty of S5P L2_NO2 (green), ex-ante relative systematic error of NO_2 MAXDOAS (red) and combined ex ante relative uncertainty (cyan). Right: standard deviation of the difference between S5P and MAXDOAS tropospheric NO2 column values (blue), ex ante uncertainty of S5P L2_NO2, random error of NO_2 MAXDOAS (red) and combined ex ante uncertainty (cyan). Dashed line indicates the product requirement.

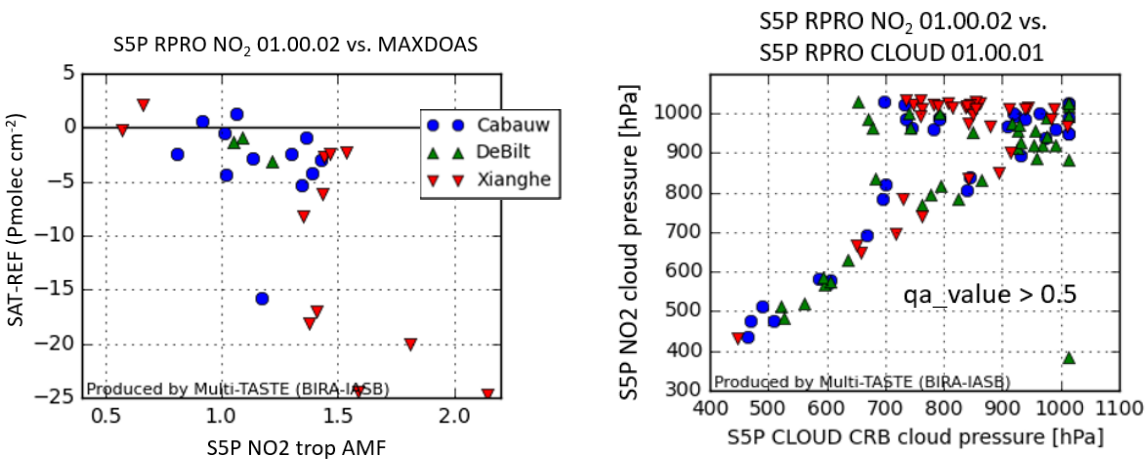

Figure 4. Left: mean difference between S5P and MAXDOAS NO_2 tropospheric column values, as a function of the S5P NO2 tropospheric air mass factor (AMF). Right: cloud pressure available in the S5P NO2 product file vs. the corresponding S5P CLOUD CRB cloud pressure.

Comparison with MAXDOAS data from the NIDFORVAL AO project

The S5PVT AO project NIDFORVAL (NItrogen Dioxide and FORmaldehyde Validation) contribute two kinds of correlative NO_2 data: tropospheric NO_2 data from UV-Vis MAXDOAS instruments, and total column NO_2 data from Pandora direct Sun instruments. Comparisons at 14 MAXDOAS have been performed on 2 months of S5P L2_NO2 RPRO (v1.0.1) tropospheric NO_2 columns (February - March 2018). Tests have been performed using different overpasses selections (averaged S5P values within 20km or closest pixel, mean ground-based column within 1h of the overpass or interpolated value at the overpass time). Selections based either on the S5P Cloud Radiance Fraction pixels in the NO_2 window (field `cloud_radiance_fraction_nitrogendioxide_window`) < 0.5 or selecting only TROPOMI pixels with `qa_value` > 0.75. Final selection is based on closest TROPOMI pixels with `qa_value` > 0.75 and interpolated ground-based columns at the overpass time. Results for tropospheric columns vs MAXDOAS are shown in Figure 5. The upper part of the figures shows the bias expressed as mean difference (absolute and relative) of the daily SAT-GB at each station and the lower part shows the corresponding scatter plot. Figure 6 presents the standard deviation of the difference with respect to the TROPOMI uncertainty estimates at each station and the precision requirement.

- Globally, TROPOMI tropospheric NO_2 columns show a negative bias (TROPOMI smaller than the ground-based values), within the 50% requirement (red lines in figures 5 and 7) and are quite variable depending on station and NO_2 level. Exceptions are very clean sites such as Cape Hedo.
- The spread of the difference between TROPOMI and MAXDOAS data exceeds the precision requirement of 0.7 Pmolec cm^{-2} at most sites (figure 6) but there is likely a large contribution of reference measurement error and comparison error to the spread. At clean sites such as Fukue and Cape Hedo, both the spread on the comparisons and the mean TROPOMI uncertainty are in agreement with the precision requirement.
- Good temporal coherence is found between TROPOMI and the MAXDOAS dataset. A correlation coefficient R of 0.76, a slope S of the orthogonal regression fit of 0.55 and an intercept I of 0.82×10^{15} molec/cm². This behavior is similar to what is achieved with OMI DOMINO v2.00 at some of the above stations (e.g., Xianghe).

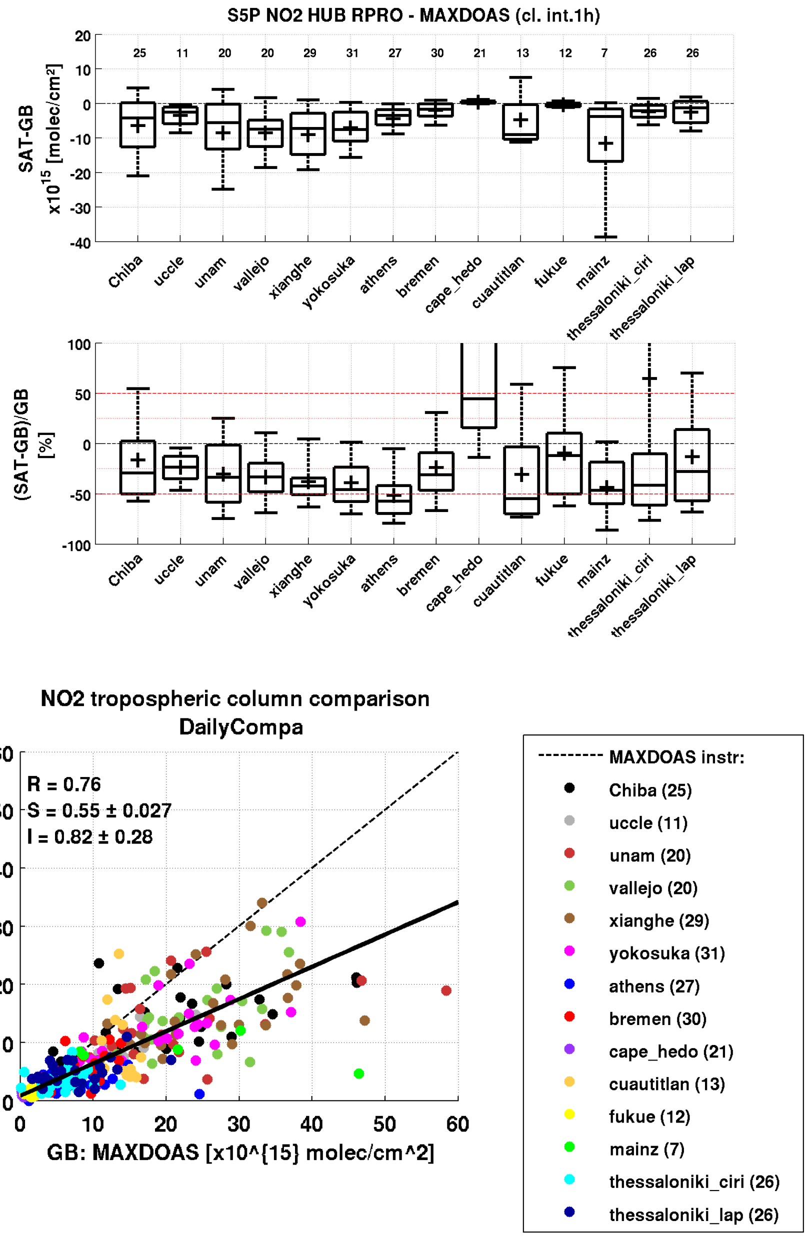

Figure 5: Top: whisker plots per station of the absolute and relative biases from the daily S5P-MAXDOAS tropospheric NO_2 comparisons. In the whisker plots, the crosses are the mean values, the lines the median, the box correspond to 25th and 75th percentiles and dotted lines show the 9th and 91th percentile. Bottom: scatter plot of the daily S5P vs MAXDOAS tropospheric NO_2 columns at each station. The numbers of comparison points are reported in the legend.

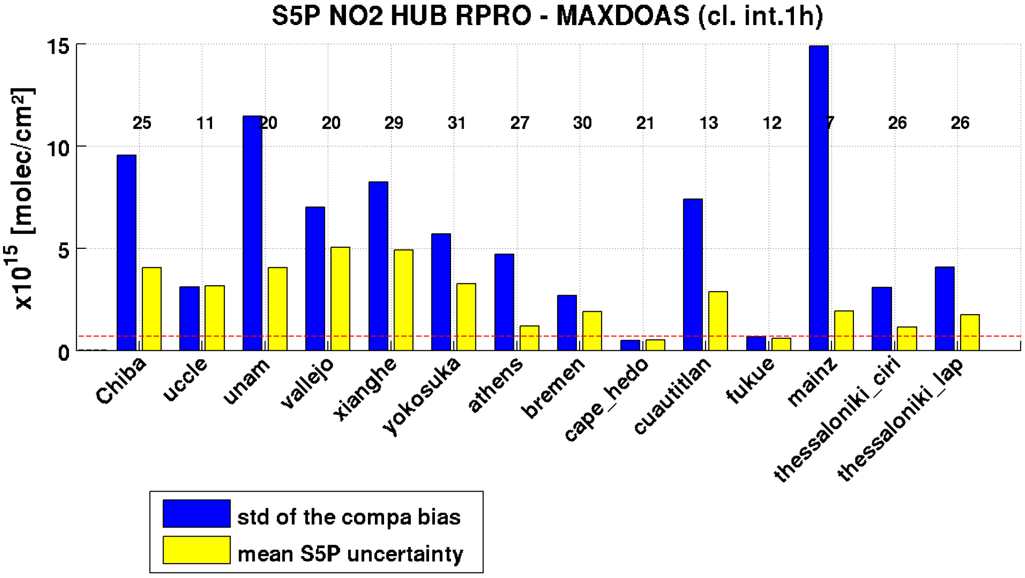

Figure 6: Standard deviation of the difference between S5P and MAXDOAS tropospheric NO_2 column values (in blue) and the mean ex ante uncertainty of the S5P NO_2 values. Red dashed line refers to the product requirement (0.7e15 molec/cm²). The numbers of comparison points at each site are reported in the figure.

Total NO_2 column

We note that no separate requirements have been formulated yet for the total NO_2 column. Therefore we take here the requirements for tropospheric NO_2. In cases with higher pollution (arguably the most relevant case for user applications), tropospheric NO_2 will be the dominant contribution to total NO_2 in winter and a significantly important contribution in summer.

Comparison with Pandora data from the NIDFORVAL AO project

Comparisons at 10 Pandora stations have been performed on 2 months of S5P L2_NO2 RPRO (v1.0.1) total NO_2 columns (February - March 2018). Tests have been performed using different overpasses selections (averaged S5P values within 20km or closest pixel, mean ground-based column within 1h of the overpass or interpolated value at the overpass time). Selections based either on the S5P Cloud Radiance Fraction pixels in the NO_2 window (field `cloud_radiance_fraction_nitrogendioxide_window`) < 0.5 or selecting only TROPOMI pixels with `qa_value` > 0.75. Final selection is based on closest TROPOMI pixels with `qa_value` > 0.75 and interpolated ground-based columns at the overpass time. Results for total columns (field `summed_total_column`) vs DirectSun data are shown in Figure 7. The upper part of the figures shows the bias expressed as mean difference (absolute and relative) of the daily SAT-GB at each station and the lower part shows the corresponding scatter plot. Figure 8 presents the spread of the differences (standard deviation of the comparison difference) with respect to the TROPOMI uncertainty estimates at each station and the precision requirement.

- Globally, TROPOMI total NO_2 columns show a negative bias (TROPOMI smaller than the ground-based values), within the 50% requirement (red lines in figures 5 and 7) and are quite variable depending on station and NO_2 level. Some exceptions are mountain/valleys sites (Izana, Davos, Innsbruck), where the conditions are difficult for the comparisons.
- The spread of the difference between TROPOMI and DirectSun data is larger than the precision requirement of 0.7 Pmolec cm^{-2} at most sites (figure 8) but there is likely a large contribution of reference measurement error and comparison error to the spread.
- Good temporal coherence is found between TROPOMI and the DirectSun dataset:
  A correlation coefficient R of 0.81, a slope S of the orthogonal regression fit of 0.67 and an intercept I of 0.38×10^{15} molec/cm².

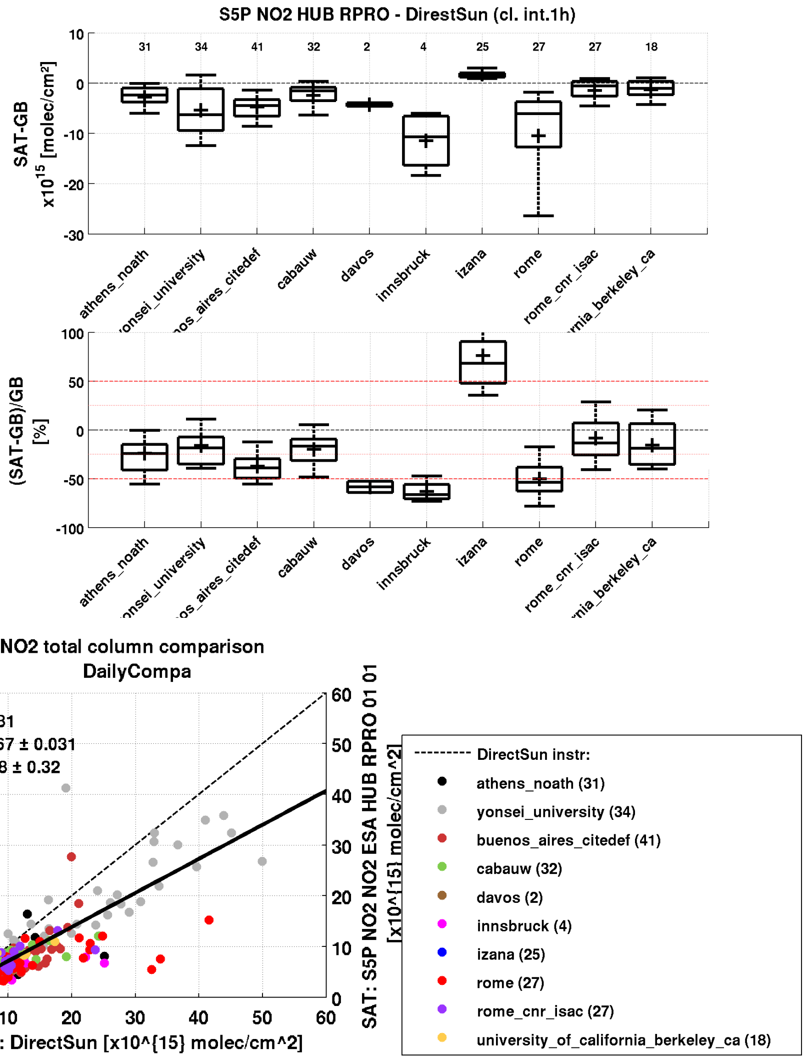

Figure 7: Top: whisker plots per station of the absolute and relative biases from the daily S5P-DirectSun total NO_2 comparisons. In the whisker plots, the crosses are the mean values, the lines the median, the box correspond to 25th and 75th percentiles and dotted lines show the 9th and 91th percentile. Bottom: scatter plot of the daily S5P vs DirectSun total NO_2 columns at each station. The numbers of comparison points are reported in the legend.

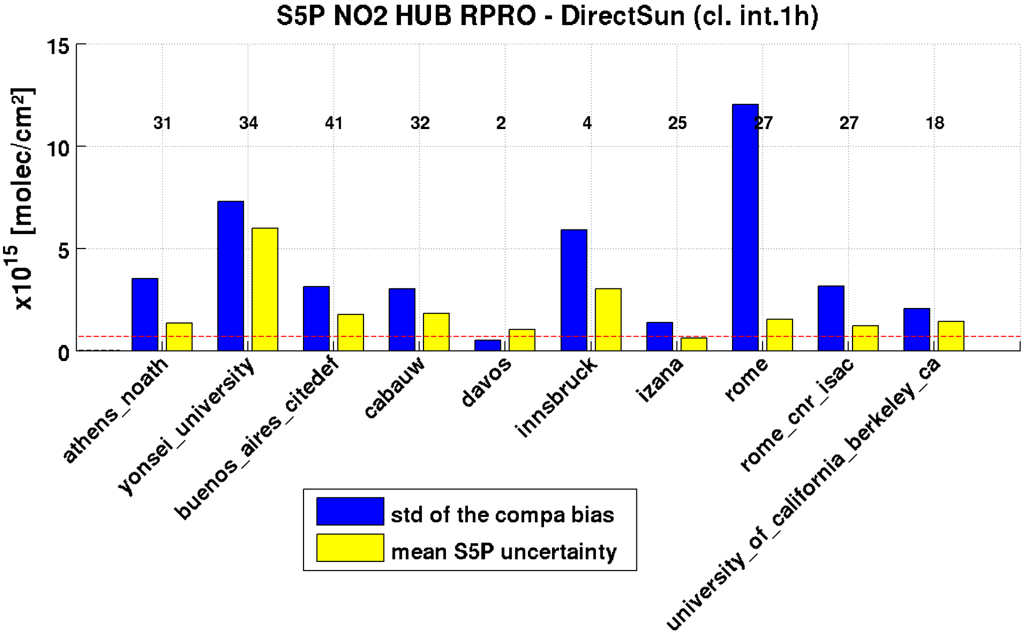

Figure 8: Standard deviation of the difference between S5P and DirectSun total NO_2 column values, in blue) and the mean ex ante uncertainty of the S5P pixels. Red dashed line indicates the product requirement (0.7e15 molec/cm²). The numbers of comparison points at each site are reported in the figure.

Acknowledgments

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The validation analyses made use of the Multi-TASTE versatile validation system operated at BIRA-IASB, of the S5P MPC Validation Data Analysis Facility (VDAF), and of the HARP Toolset maintained by s[&]t.

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