



S5P MPC VDAF

TROPOMI Validation Web Article:

Tropospheric Ozone Column

Contributing authors

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Product definition

The following table contains a description of the S5P TROPOMI processor version(s) evaluated in this report.

Processor Version	In operation from	In operation until
01.01.05	OFFL: orbit 2824, 30 Apr 2018	OFFL: orbit 7421, 20 Mar 2019
01.01.06	OFFL: orbit 7435, 21 Mar 2019	OFFL: orbit 7791, 15 Apr 2019
01.01.07	OFFL: orbit 7804, 16 Apr 2019	present

The S5P OFFL data product has the following doi: <http://doi.org/10.5270/S5P-8aqq6um>

Mission requirements for data product quality are documented 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](#)). The requirements for the systematic and random components of the uncertainty on the tropospheric ozone column are both set to a threshold of 25%.



Validation results

Sentinel-5 Precursor TROPOMI tropospheric ozone column data products (L2_O3_TCL Offline v01.01.05, v01.01.06 and v01.01.07) retrieved with the Convective Cloud Differential algorithm (CCD; source: ESA; ref: S5P-L2-IUP-ATBD-400C; issue: 1.6; date: 2018-11-07; [Sentinel-5P-ATBD-TROPOMI-Tropospheric-Ozone.pdf](#)) are compared to vertically integrated ozonesonde profile data. Those ozone profile data are measured by balloon-borne electrochemical ozonesondes launched at low latitude stations contributing to the SHADOZ network. Nine SHADOZ stations provided measurements during the period 30 April 2018 – 25 April 2019, sampling regularly all longitudes in the Tropics.

S5P CCD data products are sampled daily, each represents the three-day average of ozone partial column data between surface and 270 hPa (~10.5 km) on a 0.5° latitude by 1° longitude grid between 20°S and 20°N. SHADOZ ozonesondes are typically launched two to four times a month. They resolve the O₃ profile at 100-150 m resolution. Ozonesonde profile data are screened as in Hubert et al. (2016) and then integrated over the vertical range of the TROPOMI CCD tropospheric column. Only S5P CCD data with *qa_value* strictly larger than 0.7 are considered here, as recommended in the Product Readme File (source: ESA; ref: S5P-MPC-DLR-PRF-O3-TCL; issue: 1.0; date: 2019-02-28; [Sentinel-5P-OFFL-Tropospheric-Ozone-Product-Readme-File.pdf](#)). The SHADOZ data version used here is V06.

A reference measurement is assumed in co-location with a TROPOMI measurement provided that: (a) the SHADOZ station is located in the S5P CCD grid cell, and, (b) the ozonesonde was launched in the satellite time window. Data that do not match these criteria are not used in the calculation of the quality indicators (Figs. 2-3, Table 1). If more than one reference tropospheric ozone column falls in a co-location window, then these are averaged prior to comparison. Such a double coincidence occurs very rarely in the considered data sample. Finally, it is important to note that the spatial and temporal sampling properties of satellite and reference data records are quite different, which adds mismatch uncertainties in the comparison results on top of the combined data uncertainties.

Inspection of the S5P OFFL CCD data products (30 Apr 2018 – 25 Apr 2019, v01.01.05 + v01.01.06 + v01.01.07) and comparison to co-located ground-based reference data yield the following conclusions:

- TROPOMI captures the well-known South Atlantic ozone maximum associated with biomass burning, lightning and ozone precursors, as well as the well-known equatorial Pacific lows. S5P time series furthermore show (Fig. 1) the anticipated impact of biomass burning (high tropospheric ozone values) at Atlantic and African sites (Heredia, Paramaribo, Natal, Ascension Island, Nairobi) and signs of intense convective activity (low tropospheric ozone values) at Pacific stations (Samoa, Suva, Sepang Airport).
- The CCD algorithm requires an ample sampling of input total O₃ column data to allow a robust estimate of a reference stratospheric O₃ column. This requirement is not always fulfilled. As a result, biases of 1-2 DU between neighbouring latitude bands are found in many S5P data products. The orbital sampling by the S5P instrument progression imprints a second, somewhat more elusive spatio-temporal bias pattern that will be quantified in the near-term future.
- Co-located S5P and reference measurement time series correlate fairly well at all but one site. Pearson's skipped correlation coefficients range between 50% and 85% at individual stations, while the network average is 60% (Fig. 3, top left).
- S5P tropospheric O₃ column values are on an average larger than the ozonesonde values at 8 out of the 9 sites (Figs. 2 and 3). The mean bias over the network is +2.7 DU or +14% (Fig. 3, centre and bottom left). This is compliant with the mission requirement for a systematic uncertainty of maximum 25%.

- The half 68% interpercentile of the difference (between S5P and ozonesonde data) ranges within 2.8-7.0 DU or 12-38% (Figs. 2 and 3), and the network average is 4.2 DU or 23% (Fig. 3, centre and bottom right). An assessment of the mission requirement for the random component of the uncertainty (<25%) cannot ignore the following sources of random error: the ozonesonde instrument random uncertainty of ~5-10% and the difference in spatio-temporal sampling between S5P and ozonesonde likely contribute considerably more. Further work is needed to quantify the latter to arrive at a consolidated assessment of this requirement using ozonesonde data as a reference.

Above conclusions of TROPOMI data quality are representative of the period April 2018 to April 2019 and based on an incomplete set of reference measurements available at the time of this analysis. These conclusions need to be confirmed by a wider amount of co-locations, and extended over multiple years of data.

Known data issues

Currently, the following data quality issues are known and not covered by the quality flags. These should be kept in mind when using the tropospheric ozone column product and when interpreting preliminary validation results. These issues are described in more detail in the Product Readme File (source: ESA; ref: S5P-MPC-DLR-PRF-O3-TCL; issue: 1.0 date: 2019-02-28; [Sentinel-5P-OFFL-Tropospheric-Ozone-Product-Readme-File.pdf](#))

- Data availability is much reduced poleward of ~15° latitude in the winter hemisphere. The CCD algorithm requires a sufficient number of highly convective opaque clouds, many of which are formed in or close to the Inter Tropical Convergence Zone in the summer hemisphere.
- Filtering on *qa_value* > 0.7 does not remove all data considered bad. In some S5P products the screening procedure omits 0.5° latitude bands poleward of 15° latitude in the winter hemisphere which should have been removed. A stricter threshold may solve the issue in some cases.
- Lowering the *qa_value* threshold to values below 0.7 will increase the coverage of the S5P data record poleward of 15° latitude. However, doing so will also increase the occurrence and the magnitude of the sampling-related biases mentioned in previous section. In any case, it is not recommended to lower the screening threshold below 0.5.

Acknowledgments

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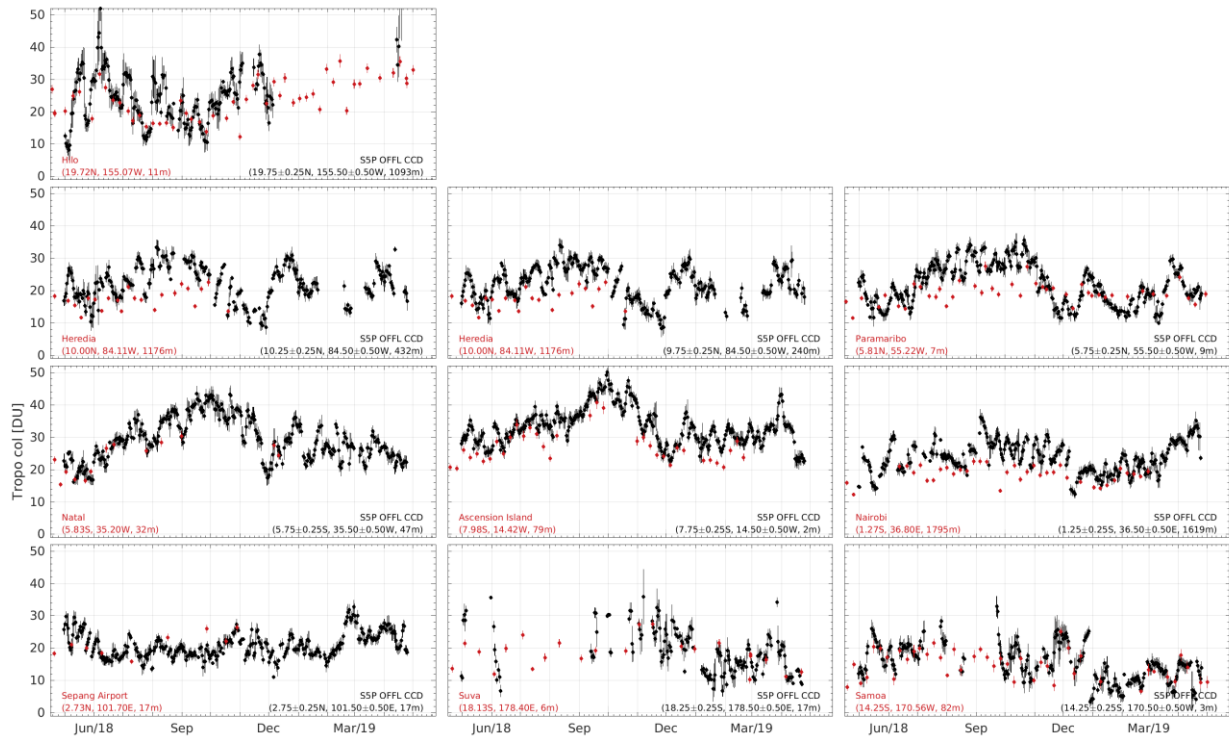


Figure 1: Time series of spatially co-located tropospheric ozone column data by ozonesonde (red) and by S5P OFFL v01.01.05+v01.01.06+v01.01.07 (black). All data have been screened as recommended by the data providers.

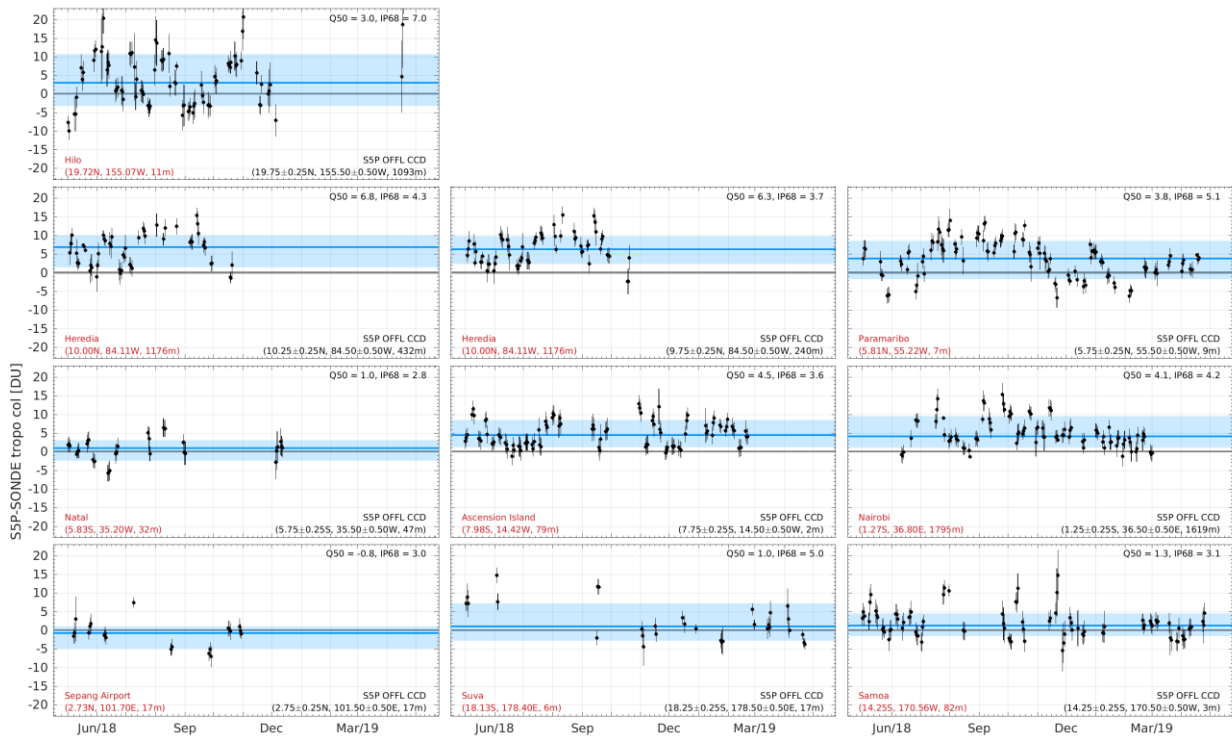


Figure 2: Time series of the absolute difference between spatially and temporally co-located S5P and ozonesonde tropospheric O₃ column data. The blue line and shaded area shows the median value and the range between the 16% and 84% percentiles. Positive values indicate a high bias of S5P w.r.t. the reference.



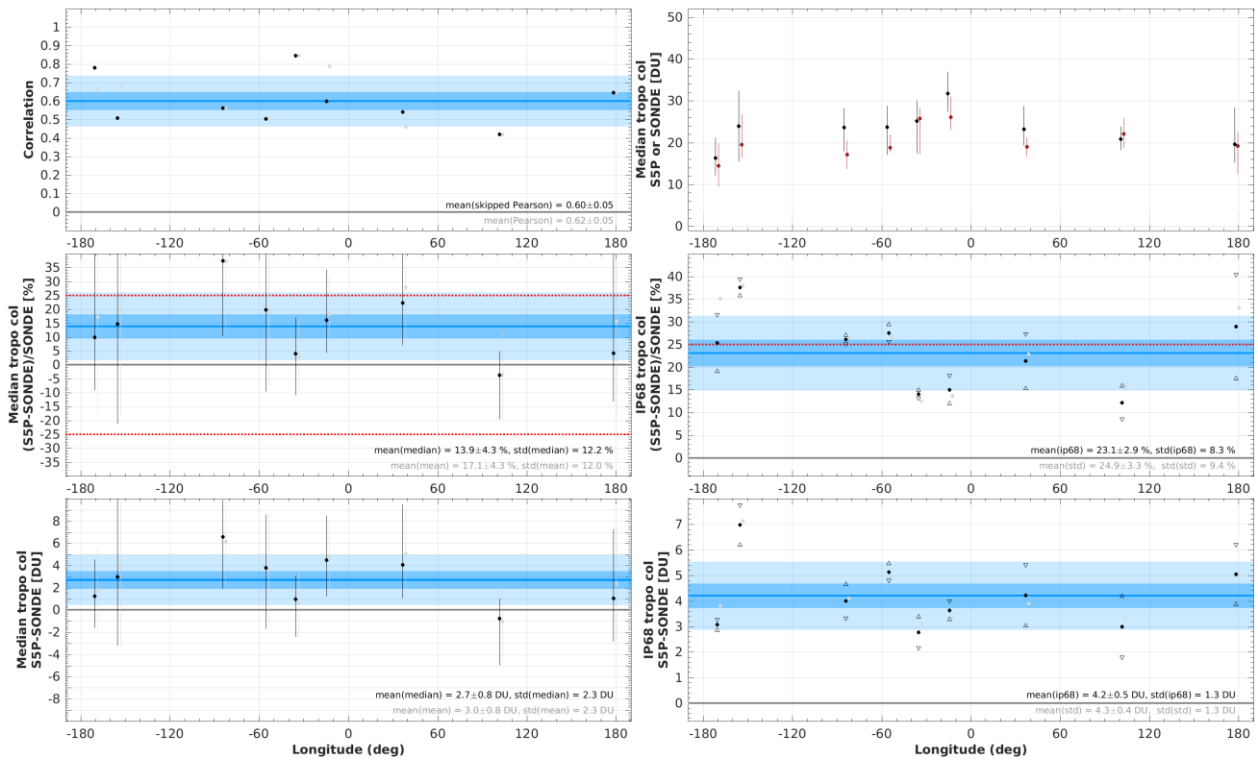


Figure 3: Overview of correlation (top left), median bias (middle & bottom left) and intercomparison spread (middle & bottom right) of S5P tropospheric ozone column data for each SHADOZ site (black markers). Black vertical bars represent the 68% interpercentile of the comparison time series. The mean, standard error of the mean (1σ) and standard deviation (1σ) of the quality indicator across the network are shown as a horizontal blue line and shaded areas.

Table 1: Overview of the location of operational SHADOZ ozonesonde stations (grouped by geophysical region), the analysis time period and three comparison statistics for the S5P OFFL v01.01.05+v01.01.06+v01.01.07 tropospheric O₃ column product. A positive bias value indicates that S5P data overestimates the values measured by the ozonesondes.

Group	SHADOZ site	Lon.	Lat.	Alt.	Analysis period	Correlation	Bias	Comparison spread
Hawaii	Hilo	155.1°W	19.7°N	11 m	2018/04 - 2019/04	0.51	3.0 DU 14.6 %	7.0 DU 37.5 %
Equatorial Americas	Heredia† (Costa Rica)	84.1°W	10.0°N	1176 m	2018/04 - 2018/10	0.56	6.5 DU 37.5 %	4.0 DU 26.1 %
	Paramaribo	55.2°W	5.8°N	7 m	2018/04 - 2019/04	0.50	3.8 DU 19.9 %	5.1 DU 27.5 %
Atlantic & Africa	Natal	35.2°W	5.8°S	32 m	2018/04 - 2018/12	0.85	1.0 DU 8.6 %	2.8 DU 21.4 %
	Ascension Island	14.4°W	8.0°S	79 m	2018/04 - 2019/02	0.60	4.5 DU 16.1 %	3.6 DU 15.0 %
	Nairobi	36.8°E	1.3°S	1795 m	2018/04 - 2019/02	0.54	4.1 DU 22.3 %	4.2 DU 21.3 %
East Indian & Western Pacific	Sepang Airport (Kuala Lumpur)	101.7°E	2.7°N	17 m	2018/04 - 2018/10	0.42	-0.8 DU -3.7 %	3.0 DU 12.2 %
	Suva (Fiji)	178.4°E	18.1°S	6 m	2018/04 - 2019/04	0.65	1.0 DU 4.2 %	5.0 DU 28.9 %
	Samoa (Pago Pago)	170.6°W	14.2°S	82 m	2018/04 - 2019/04	0.78	1.3 DU 9.9 %	3.1 DU 25.3 %
Mean across network :					2018/04 - 2019/04	0.60	2.7 DU 13.9 %	4.2 DU 23.1 %

† Heredia is located on the boundary of two S5P CCD cells, so co-locations are formed for both cells. The resulting quality indicators are averaged to obtain one reported value for the Heredia station.

