Six years of Sentinel-5p TROPOMI operational ozone profiling: Retrieval approach and geophysical validation

Arno Keppens (BIRA-IASB), Serena Di Pede (KNMI), et al.

Motivation

- Based on Keppens, et al., AMT, 2024, published yesterday
  https://doi.org/10.5194/amt-17-3969-2024
- Extended to 6+ years of data:
  May 2018 – May 2024
- Added sat-sat intercomparison,
  as foreseen in current ATM-MPC CCN
- 10’ flyover

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6 years of Sentinel-5P TROPOMI operational ozone profiling and geophysical validation using ozonesonde and lidar ground-based networks

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Abstract. The Sentinel-5 Precursor (S5P) satellite operated by the European Space Agency has carried the TROPOspheric Monitoring Instrument (TROPOMI) on a Sun-synchronous low-Earth orbit since 13 October 2017. The S5P mission has acquired more than 5 years of TROPOMI nadir ozone profile data retrieved from the level 0 to 1B processor version 2.0 and the level 1B to 2 optimal-estimation-based processor version 2.4.0. The latter is described in detail in this work, followed by the geophysical validation of the resulting ozone profiles for the period May 2018 to April 2023. Comparison of TROPOMI ozone profile data to co-located ozonesonde and lidar measurements used as references concludes to a median agreement better than 5 % to 10 % in the troposphere. The bias goes up to −15 % in the upper stratosphere (35–45 km) where it can exhibit vertical oscillations. The comparisons show a dispersion of about 30 % in the troposphere and 10 % to 20 % in the upper troposphere to lower stratosphere and in the middle stratosphere, which is close to mission requirements. Chi-square tests of the observed differences confirm on average the validity of the ex ante (prognostic) satellite and ground-based data uncertainty estimates in the middle stratosphere above about 20 km. Around the tropopause and below, the mean chi-square value increases up to about four, meaning that the ex ante TROPOMI uncertainty is underestimated. The information content of the ozone profile retrieval is characterised by about five to six

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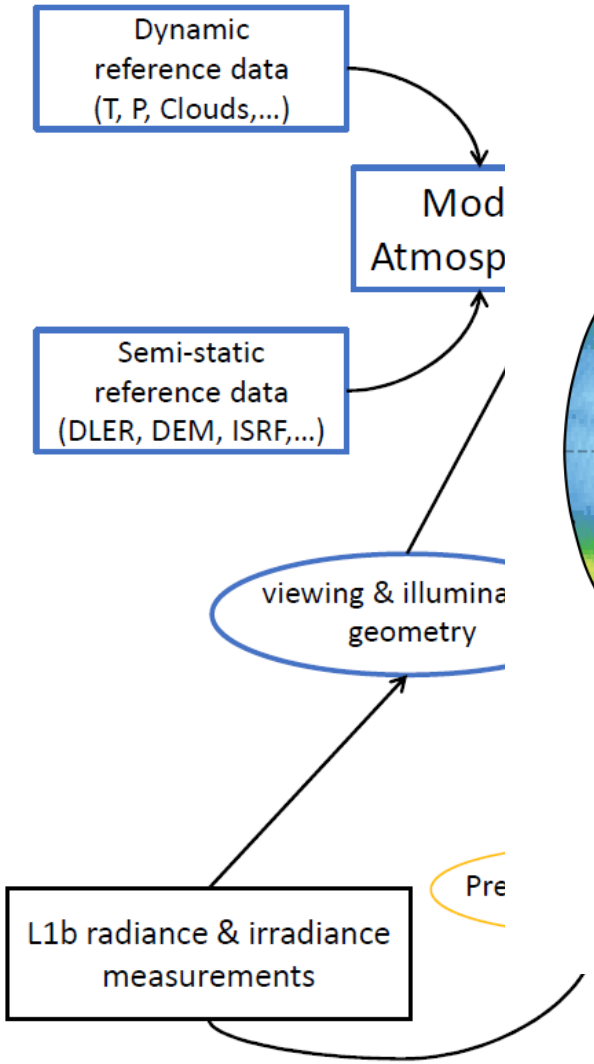
- BELSPO/ProDex TROVA 3
- GAW, NDACC, SHADOZ, TOLNET instrument PIs and staff

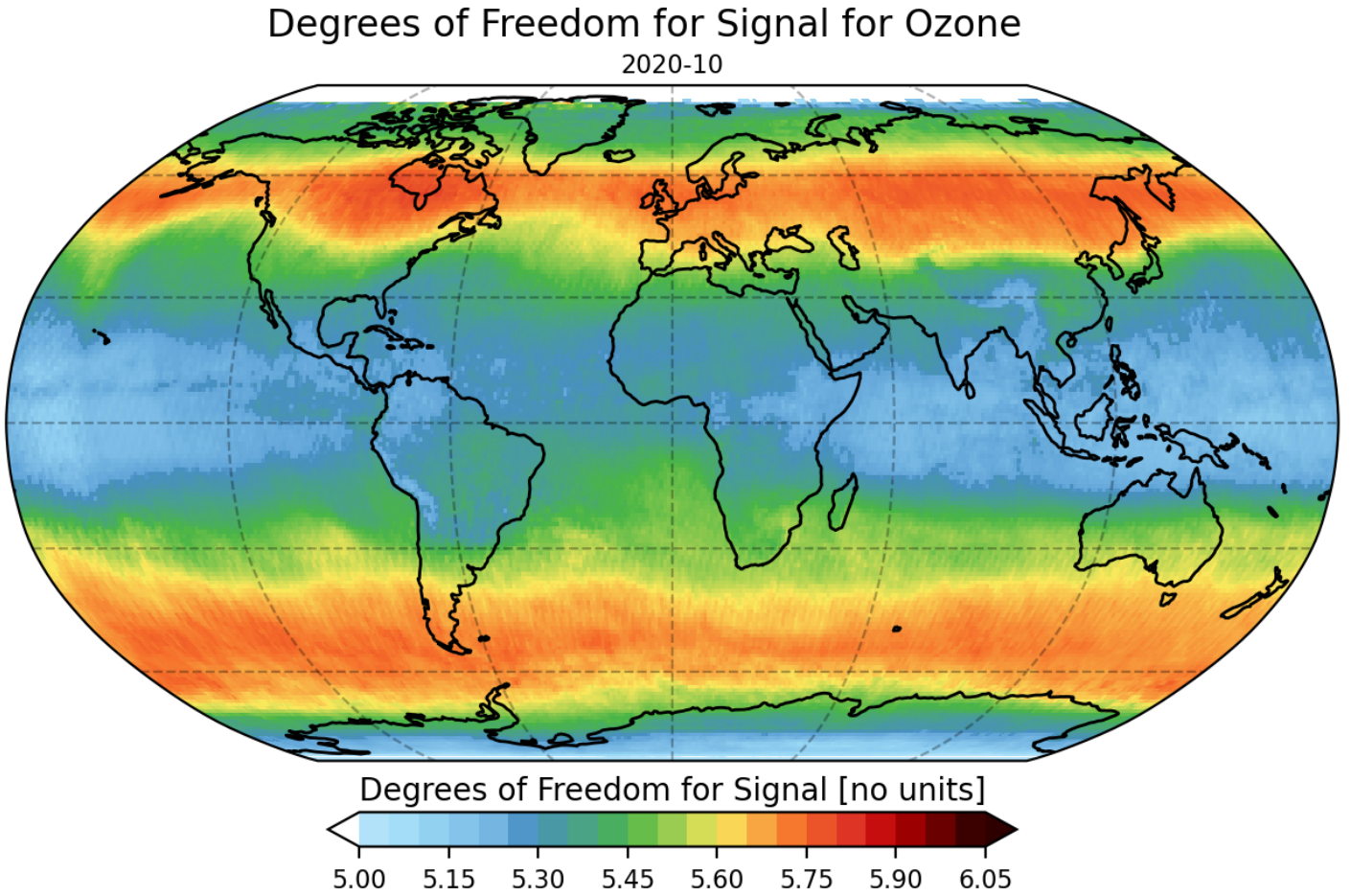
TROPOMI operational ozone profile data

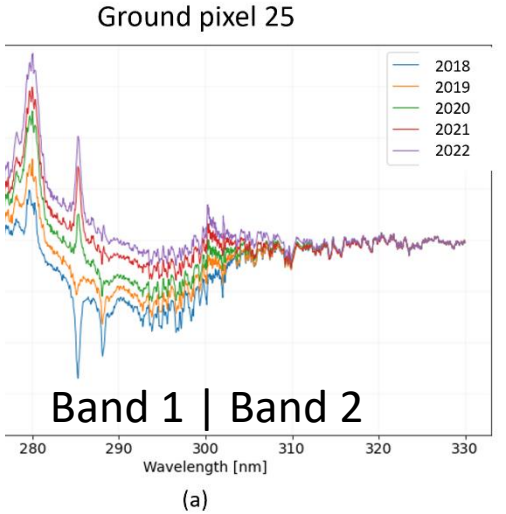
- Full RPRO/OFFL time series from KNMI's NL-L2 v2.4-6 processing
- Ozone profile as "mole_concentration_of_ozone_in_air" on 33 levels
- Derived product consisting of six integrated subcolumns (see talk 5.1.7 by S. Di Pede)

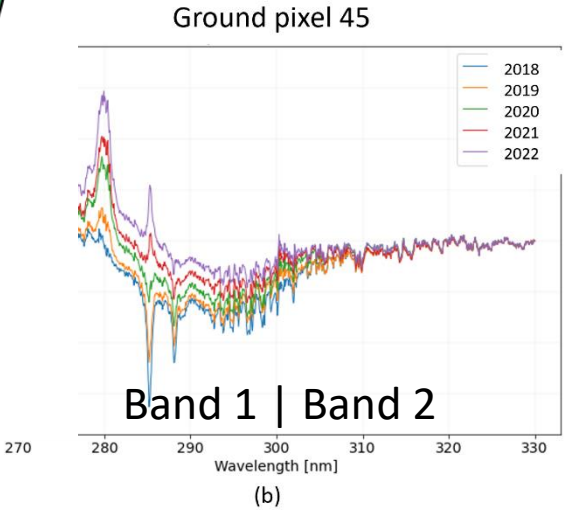
Date	Operational processing change
2018/04/30	RPRO v02.04 start date using soft-calibration v2
2019/08/06	TROPOMI pixel resolution change
2022/07/17	OFFL v02.04 start date using soft-calibration v1
2022/07/25	RPRO end date
2022/09/08	QA value threshold update
2023/01/15	OFFL soft-calibration update to v2
2023/03/15	NRTI checkerboard pattern (v02.05)
2023/11/29	NRTI & OFFL update to v02.06 (minor)

TROPOMI operational ozone profile retrieval



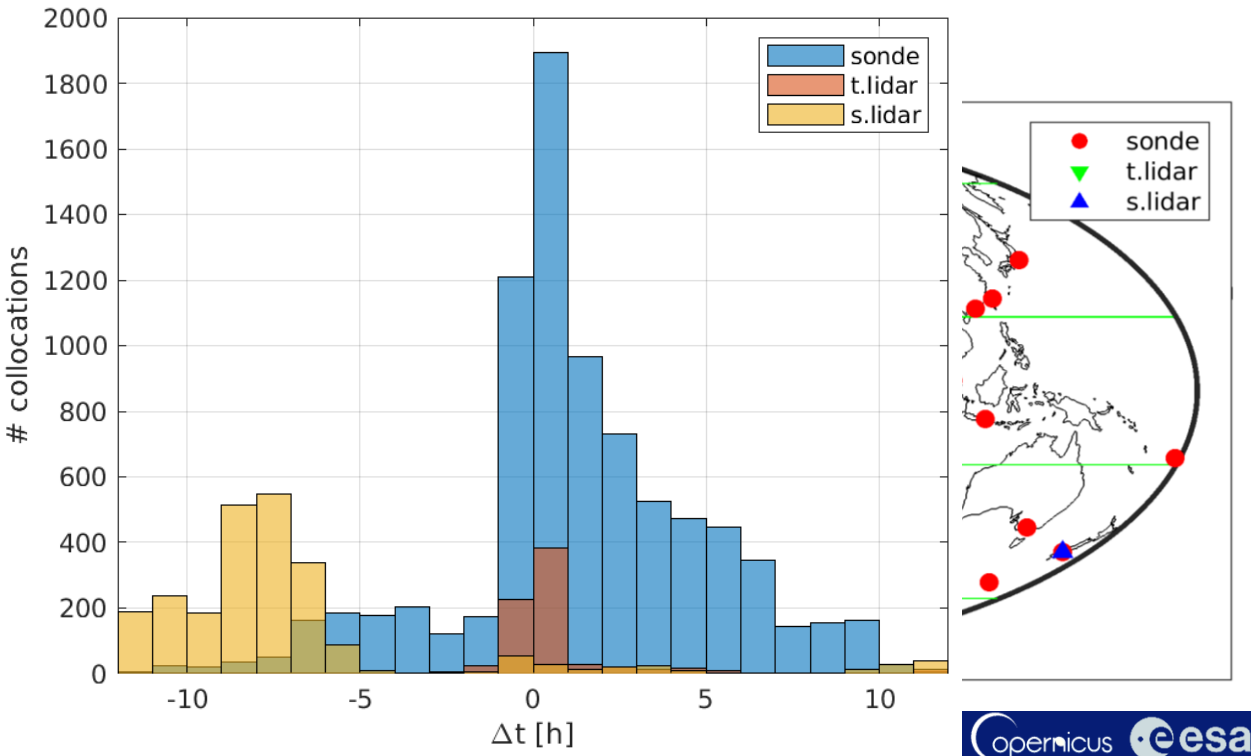




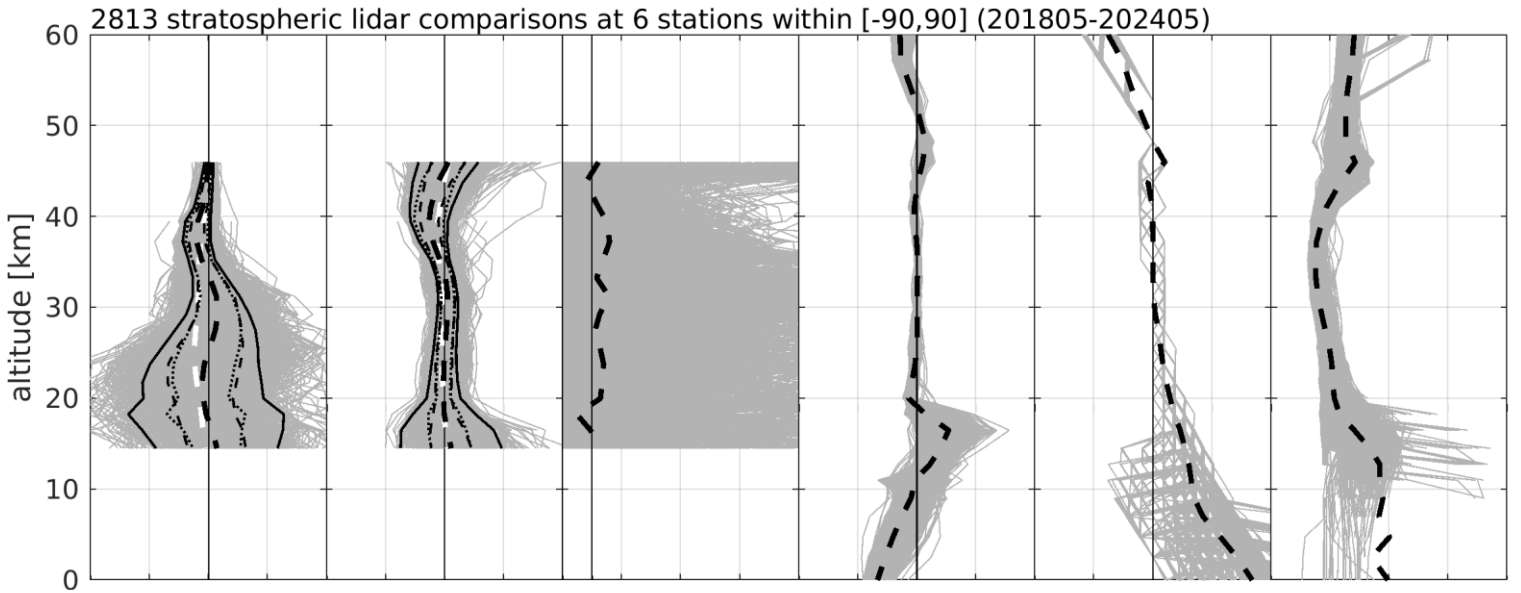


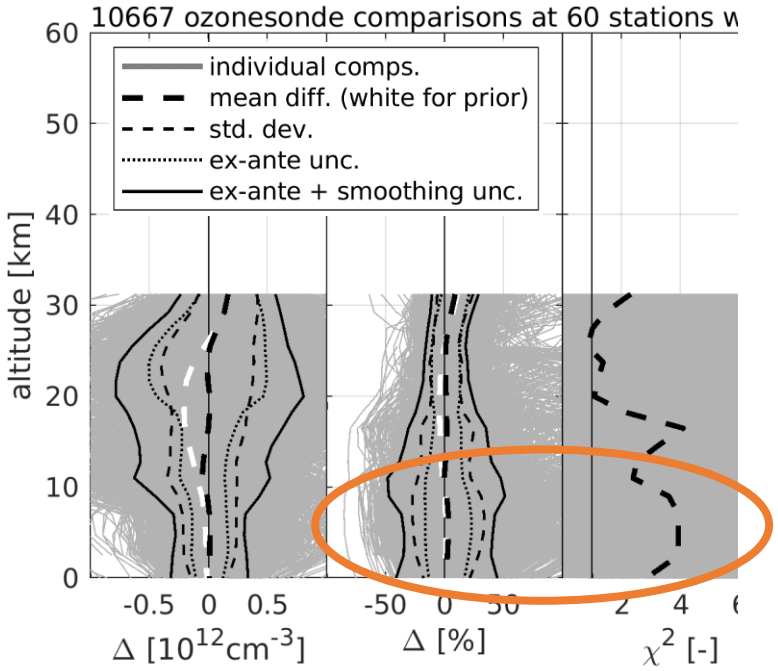
Ground-based validation: data & settings

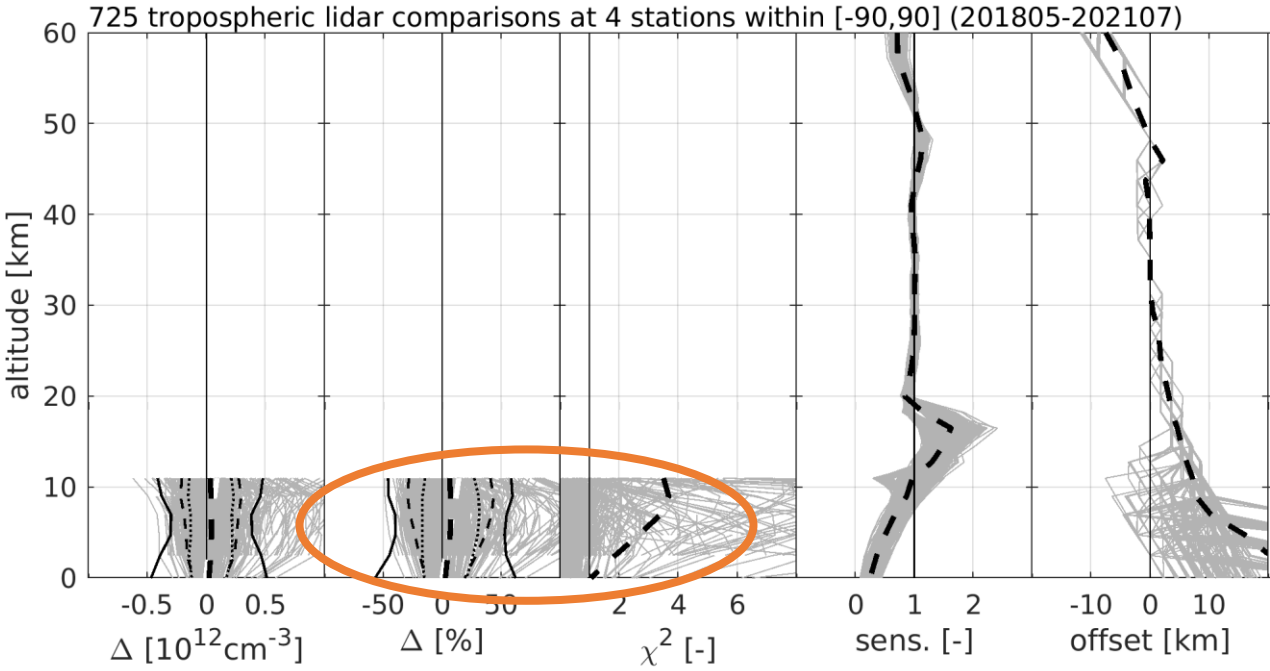
- TROPOMI O3_PR for qa_value > 0.5
- Validation data (FRM) through EVDC
  - NDACC/SHADOZ/WOUDC networks + MATCH campaign ozonesonde
  - NDACC/TOLNET tropospheric and stratospheric lidar
- Co-location
  - same day (±12h)
  - overpass pixel (AVS: “point-in-area”)
- 14K+ co-located data pairs
  - 60 ozonesonde stations
  - 10 lidar stations
- Mass-conserved regridding and averaging kernel smoothing of FRM data (Keppens et al., 2019)



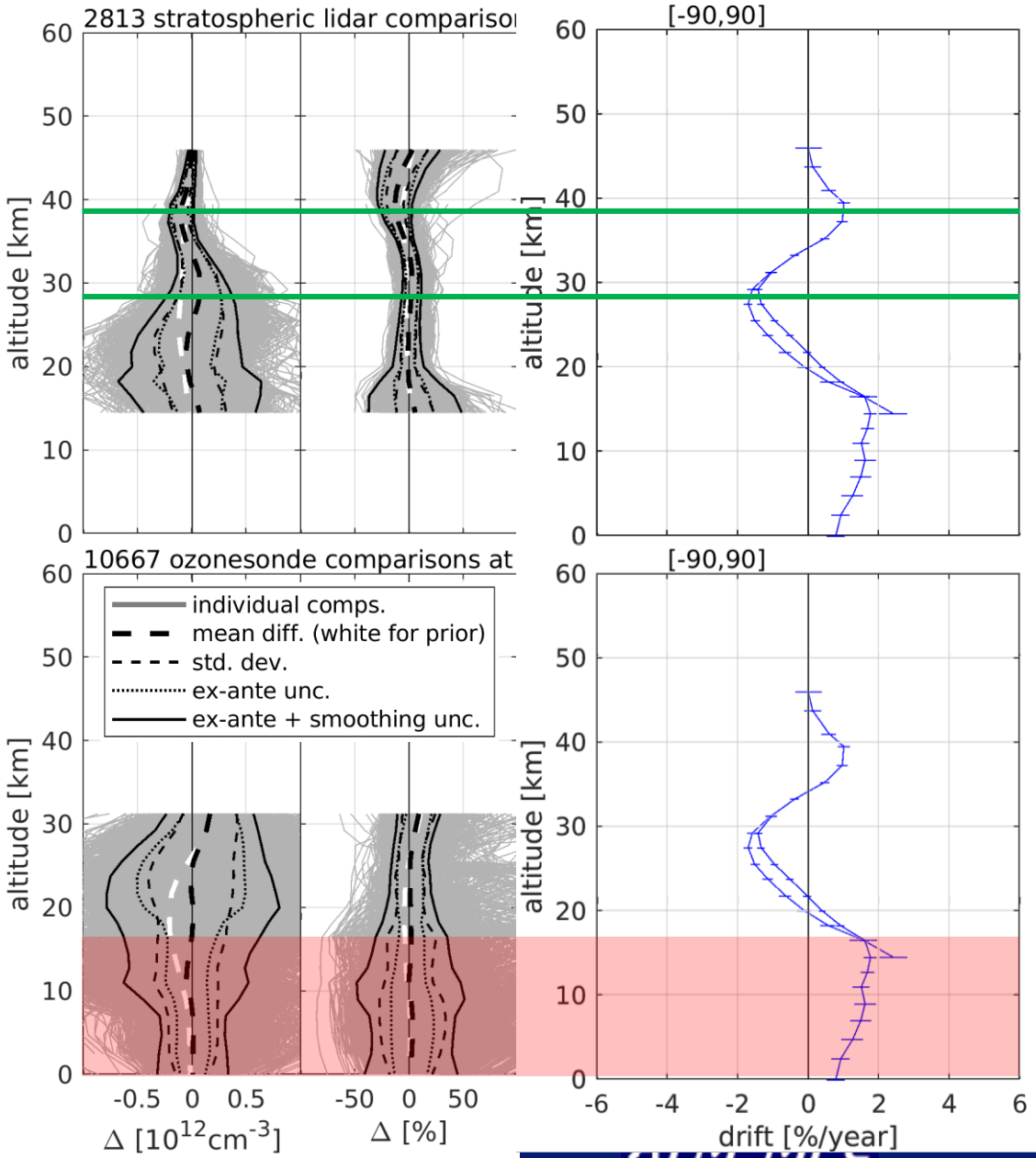
FRM comparisons and information content





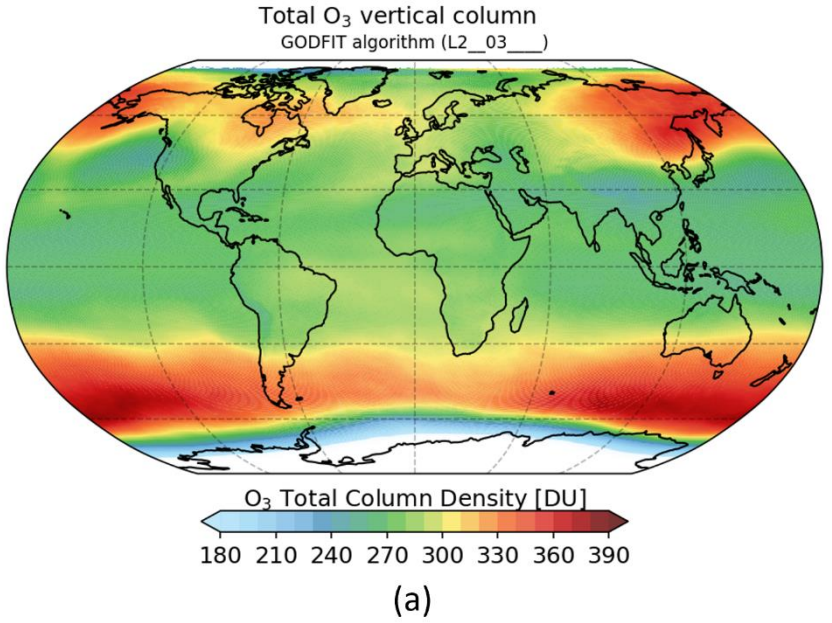


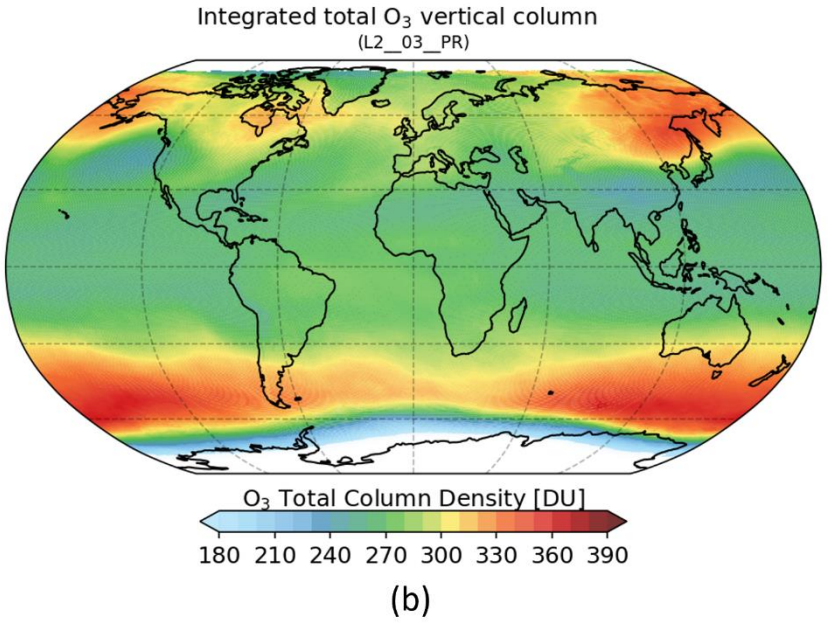
FRM comparisons: drift

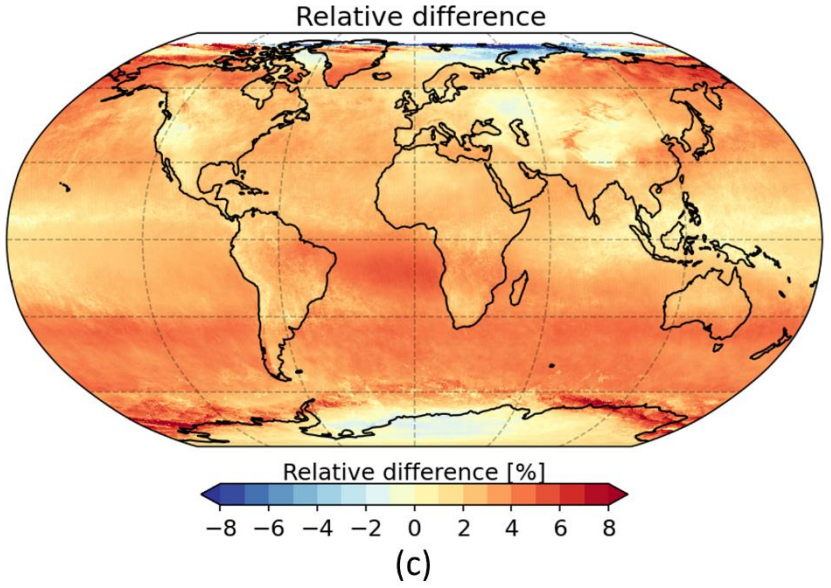


- Decreasing stratospheric bias (oscillations)
- Increasing positive tropospheric bias
- Insignificant vertically integrated drift

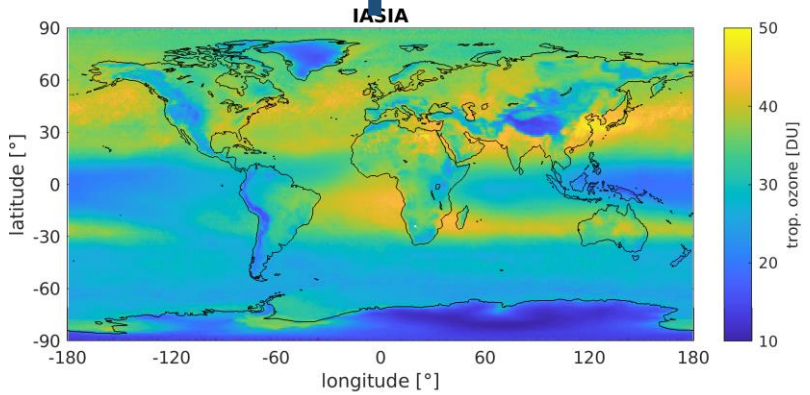
L3 total column intercomparisons (Oct. 2020)

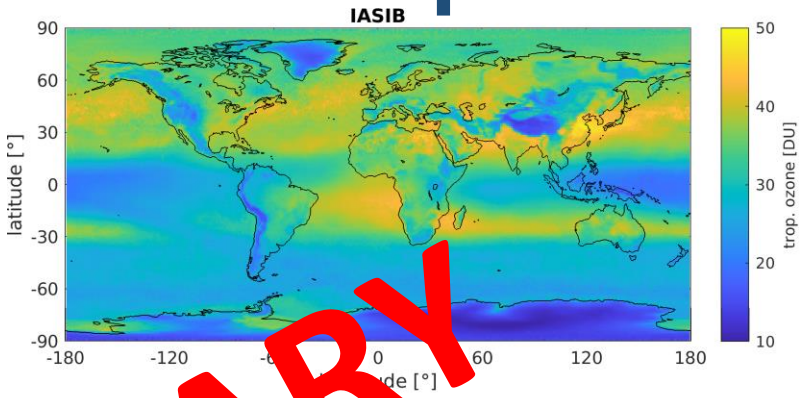


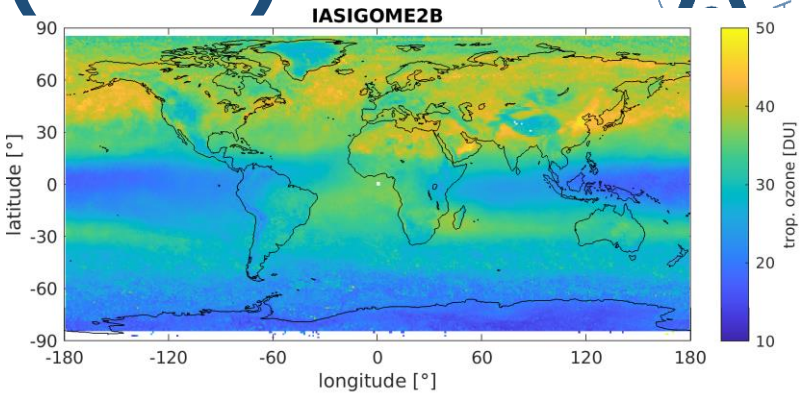


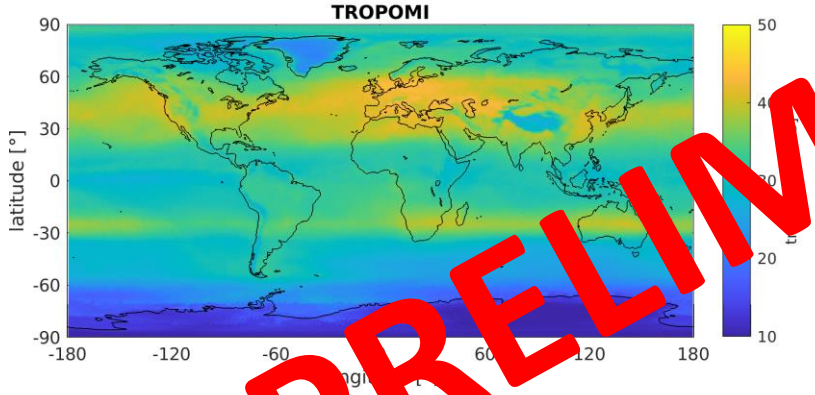


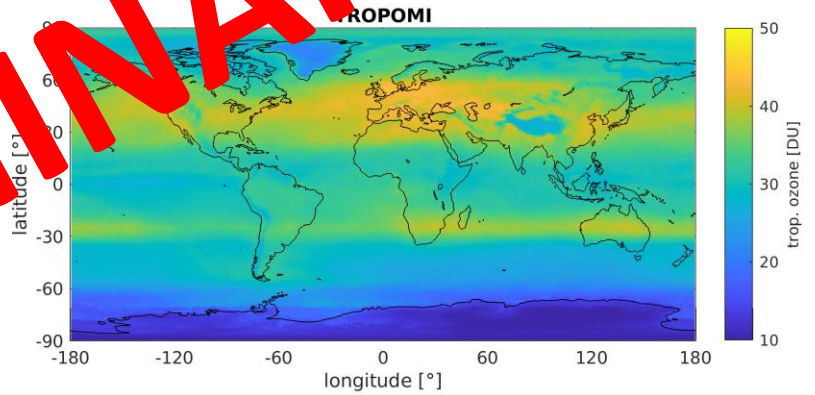
L3 tropo-column intercomparisons (2019)

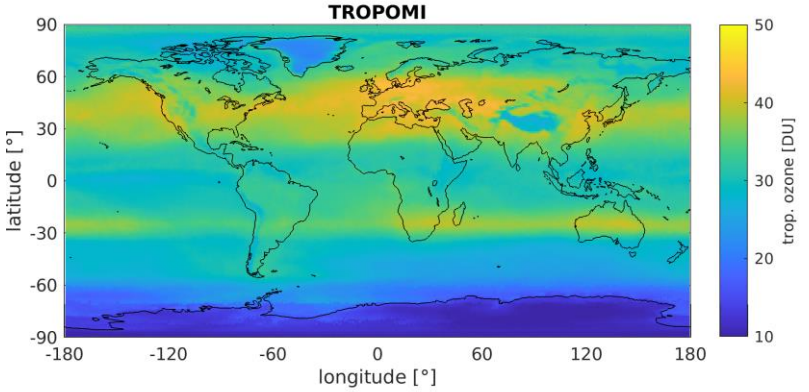


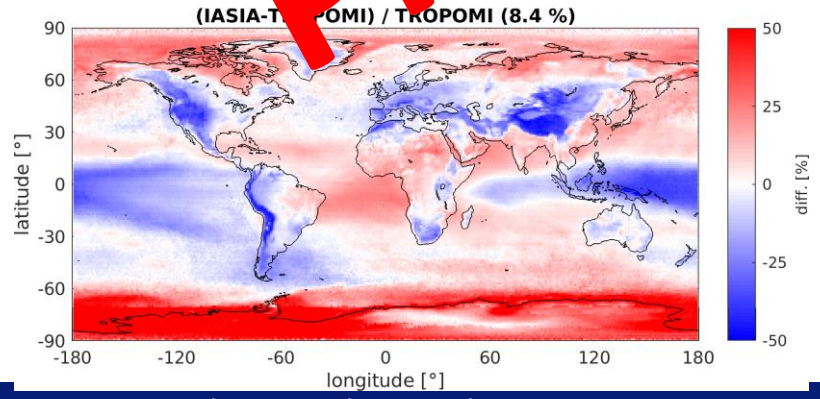


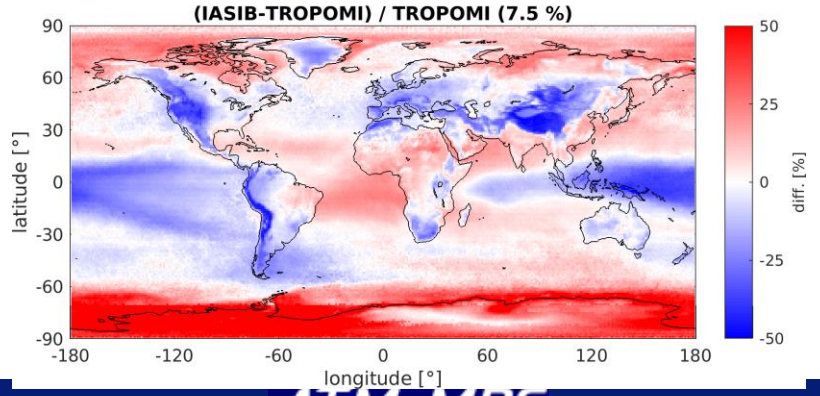


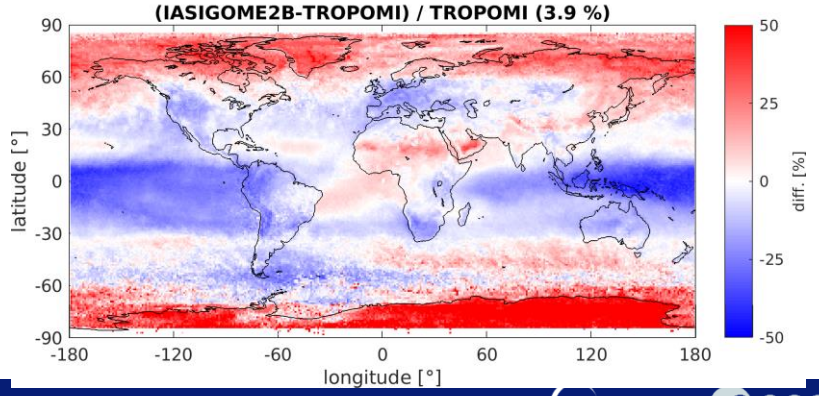












PRELIMINARY

Key results

- 5-6 pieces of independent information, with optical path dependence and neg. drift
- Sensitivity: above 1 peak in UTLS, below 0.5 at surface
- Effective vertical resolution: 7 (at 35 km) to 15 km (UTLS)
- Retrieval altitude offset: about 10 km towards surface and TOA
- Overall bias: 5-10 %, vertical oscillations in stratosphere (-15 % max) for low SZA
- Dispersion: 20-30 % below TP, 5-10 % above
- Ex-ante uncertainty underestimated (factor of 2) below TP
- Drift: latitude-dependent, highest in mid-lat. troposphere, negative in stratosphere
- Negligible integrated drift
- Integrated profile slightly underestimates total column ozone (~5 %)
- Slight striping along orbit
- Reduced retrieval quality for high SZA and surface albedo (around Antarctic)
- Mostly fully compliant with mission requirements

ATMOS 2024 recommendations

- Coincident observation exploitation: L1 joint retrieval, L2 data fusion, L3 data merging, AND validation focus on (vertically resolved) chi-square testing from FRM and triple co-locations from both FRM and satellites
  cf. ATMOS 2021 R4 / R36 / R38; also see ISSI special issue on “Remote Sensing In Climatology – ECVs and their Uncertainties” (Springer Surveys in Geophysics)

- Active data / analysis contributions to tropospheric and stratospheric ozone assessments
  cf. ATMOS 2021 R5 / R37