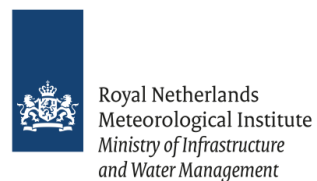


Quality assessment of the Sentinel-5p TROPOMI operational ozone profile data

A. Keppens, J.-C. Lambert, D. Hubert, S. Compernelle, T. Verhoelst, S. Niemeijer, A. M. Fjaeraa, M. ter Linden, M. Sneep, J. de Haan, P. Veeffkind, A. Dehn, and the CHEOPS-5p validation team (add. incl. G. Ancellet, D. Balis, A. Delcloo, V. Duflot, S. Godin-Beekmann, T. Leblanc, T. Stavrakou, W. Steinbrecht, R. Stübi, and A. M. Thompson)



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- ESA/Copernicus ATM Mission Performance Cluster
- CHEOPS-5p validation team: G. Ancellet, D. Balis, A. Delcloo, V. Duflot, S. Godin-Beekmann, T. Leblanc, W. Steinbrecht, R. Stübi, A. M. Thompson
- BELSPO/ProDex TROVA-E2 CHEOPS-5p
- GAW, NDACC, SHADOZ, TOLNET instrument PIs and staff



TROPOMI operational ozone profile data

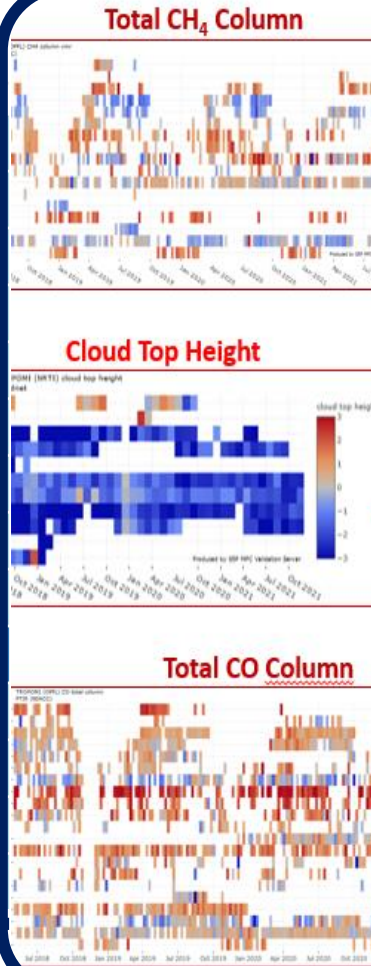
- Full ozone profile as “mole_concentration_of_ozone_in_air” on 33 vertical levels
- Derived product consisting of six integrated subcolumns (~ 1 DFS)
- Pixel co-adding to spatial resolution of 28 x 28 km² (nadir)
- Optimal estimation retrieval preceded by soft-calibration to match wavelength bands 1-2
- Implemented into S5P Payload Data Ground Segment (PDGS) in November 2021
- Processor NL-L2 v2.3.1 since November 16 (OFFL) and 24 (NRTI), 2021, from L1B v2.0.0
- Processor NL-L2 v2.4.0 since July 17 (OFFL) and 20 (NRTI), 2022, from L1B v2.1.0
- QA-value threshold update on Sept. 8, 2022
- Full reprocessing using NL-L2 v2.4.0 and paper writing ongoing...

TROPOMI O3_PR QA approaches

S5P - Mission Performance Centre - Level 2 Quality Control Portal

Previous day Next day

AER_AI
AER_LH
CH4___
CLOUD_
CO___
FRESCO
HCHO___
NO2___
O3___
O3__PR
O3_TCL
SO2___
NP_BD3
NP_BD6



Tropospheric NO₂ Column

Total NO₂ Column

Home Search VDAF Server Log



VALIDATION FACILITY

SENTINEL-5 PRECURSOR MISSION PERFORMANCE CENTRE



The Sentinel-5P Validation Data Analysis Facility (VDAF) portal is the public entry point to the Routine Operations Validation Service for TROPOspheric Monitoring Instrument (TROPOMI).

Launched on 13 October 2017 on board of the ESA/Copernicus Sentinel-5 Precursor satellite, TROPOMI measures each day the global distribution of atmospheric trace gases and aerosols for a better understanding of air quality, the ozone layer, atmospheric chemistry and transport, ultraviolet radiation, and climate change.

Since the start of S5P Routine Operations in 2018, the S5P Mission Performance Centre (MPC) provides the operational validation service for the Level-1 and Level-2 data products generated by the Near Real Time (NRTI) and Offline (OFFL) processors. Procured by an international consortium coordinated by the Royal Belgian Institute for Space Aeronomy (BIRA-IASB) and supervised by ESA and KNMI, the S5P Routine Operations Validation Service integrates validation monitoring with the Automated Validation Server (VDAF-AVS), in-depth studies carried out by the S5P MPC, ad hoc support from S5P Validation Team (S5PVT) AO projects, and feedback from the Copernicus Atmosphere Monitoring Service (CAMS) at ECMWF.

Sentinel-5P TROPOMI data users are encouraged to consult the latest issue of the quarterly Routine Operations Consolidated Validation Report (ROCVR), and to apply data filtering and other recommendations provided in the Product Readme Files (PRF) delivered with the S5P data products.

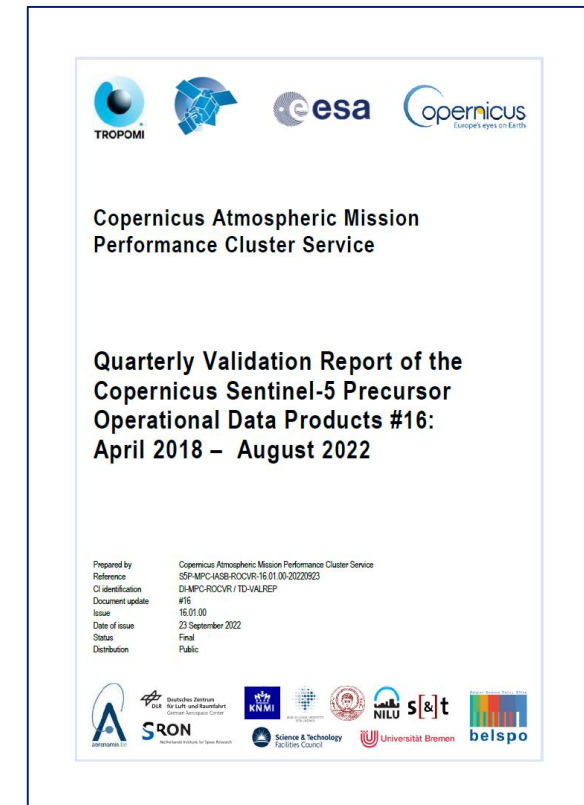


TROPOMI O3_PR QA approaches

- ESA/Copernicus S5P/ATM MPC
 - L2 quality control portal (KNMI) <http://mpc-l2.tropomi.eu/>
 - Automated Validation Server (s[&t) <http://mpc-vdaf-server.tropomi.eu/>
 - Validation Data Analysis Facility (BIRA-IASB) <https://mpc-vdaf.tropomi.eu/>
- S5PVT
 - BELSPO/ProDex TROVA-E2 CHEOPS-5p

Results summarized in 3-monthly ROCVR, reporting on...

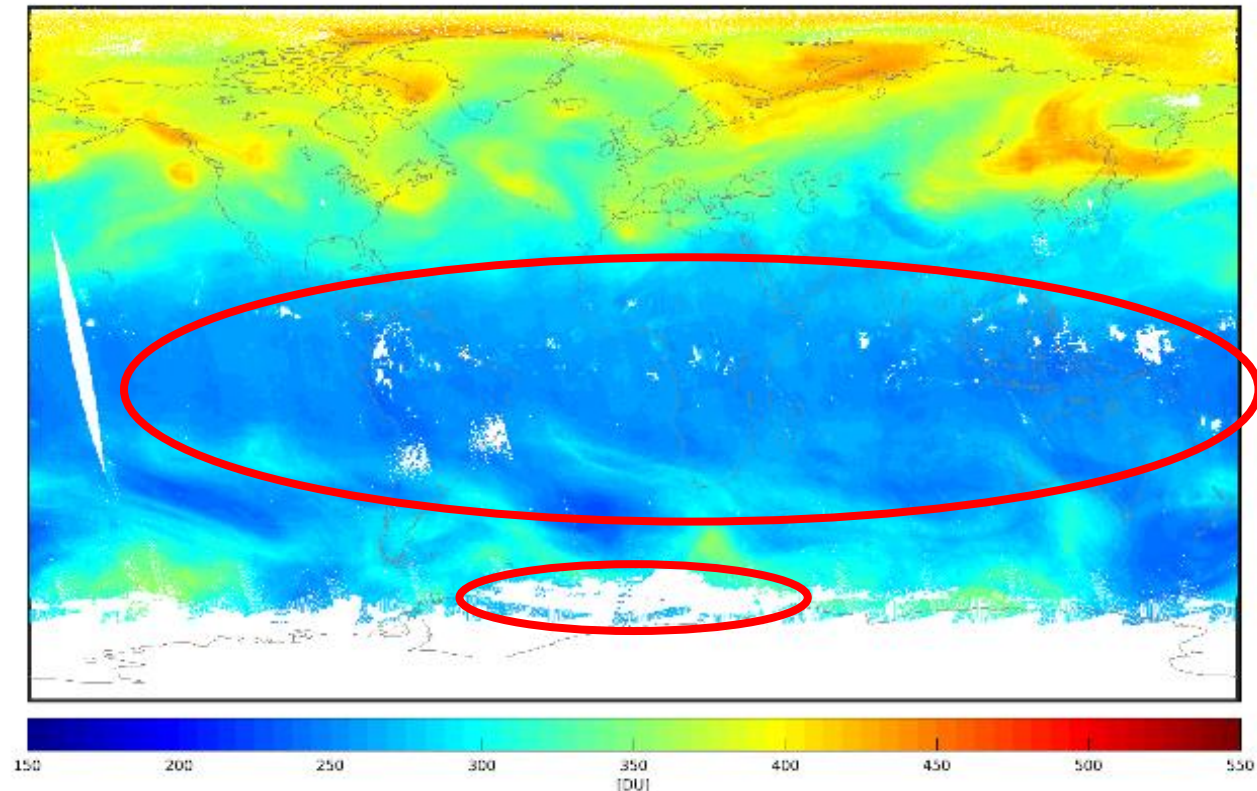
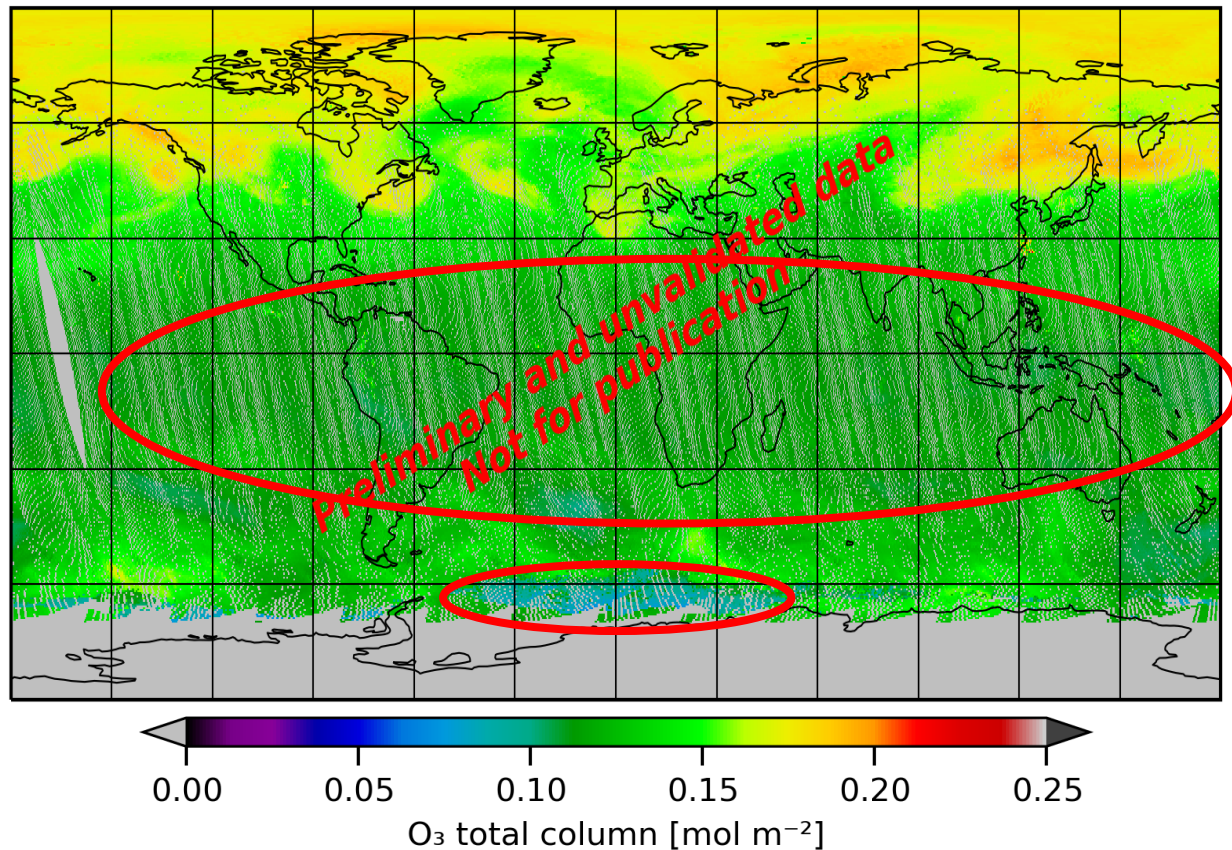
- D/W/M maps: global, Europe, North America
- Consistency checks with total and tropospheric ozone data
- Data & information content studies
- Ground-based comparisons w.r.t. influence quantities
- Delta-validation of data reprocessings



Daily global maps

Integrated ozone profile for OFFL product, April 29, 2022

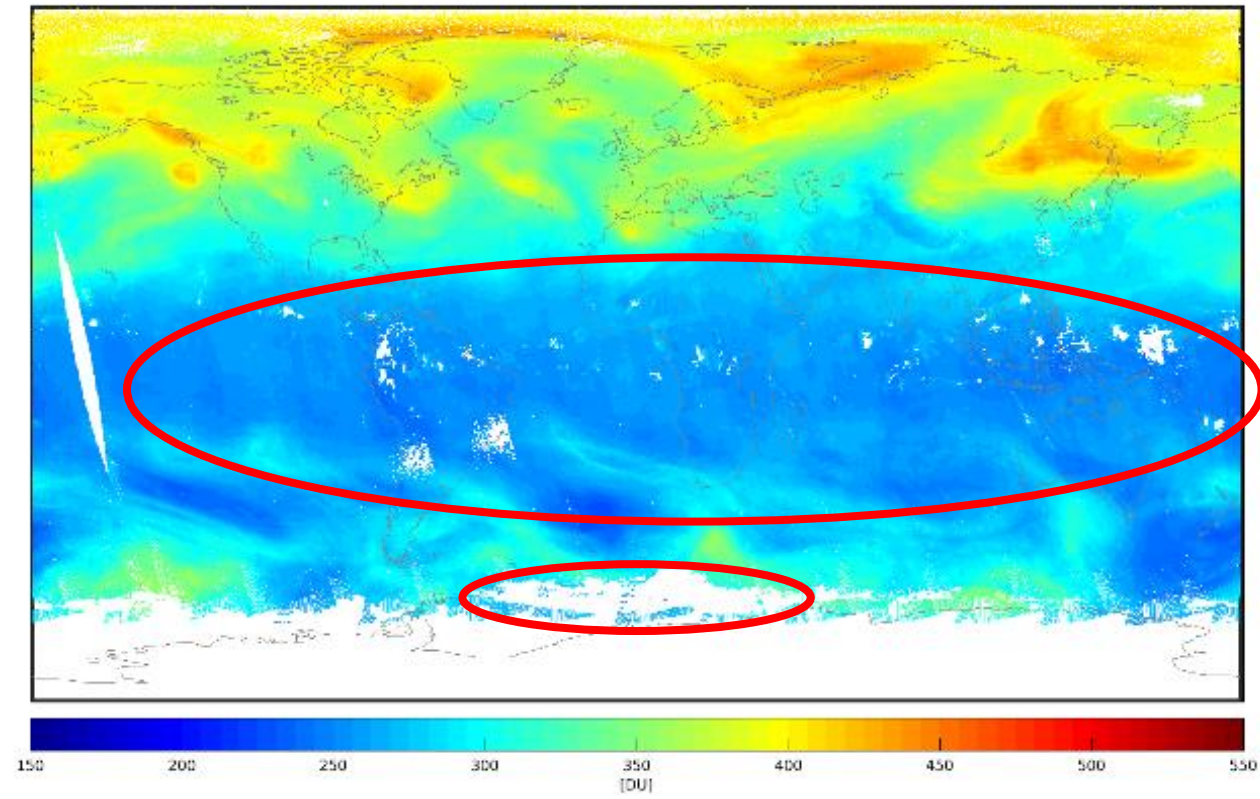
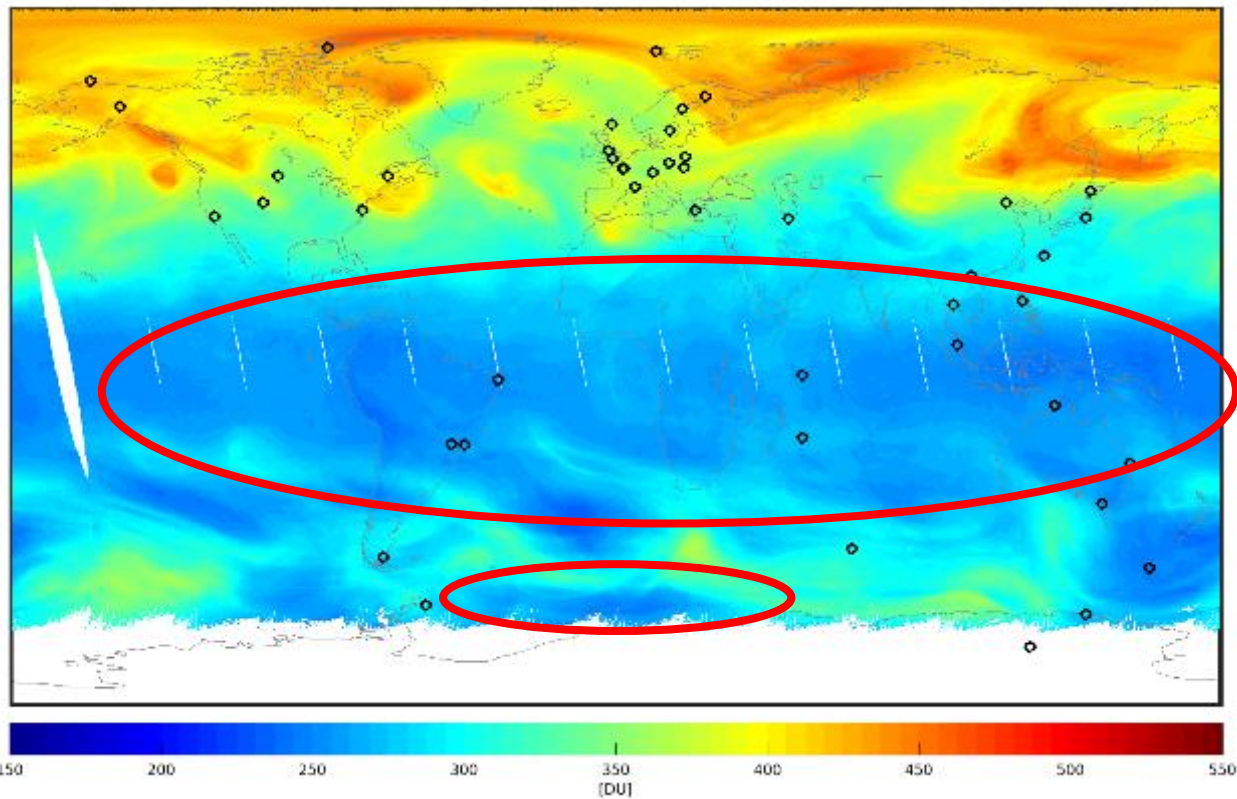
- L2 quality control portal (KNMI): without QA flagging
- Validation Data Analysis Facility (BIRA-IASB): with QA flagging



Daily global maps: VDAF consistency checks

Total ozone for OFFL products, April 29, 2022

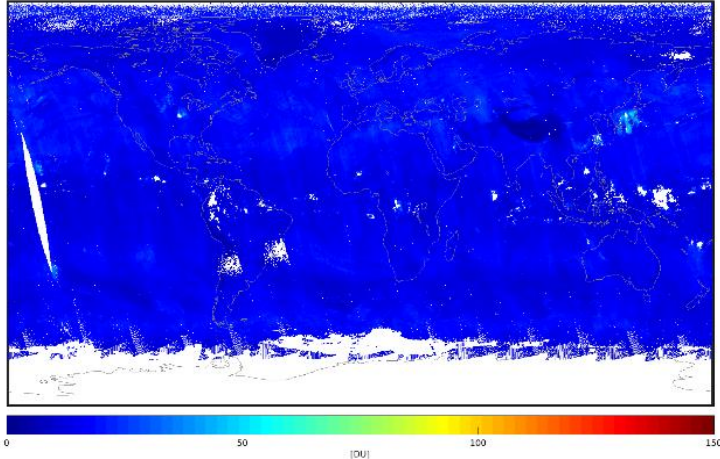
- L2_O3 with QA flagging
- L2_O3_PR vertically integrated with QA flagging



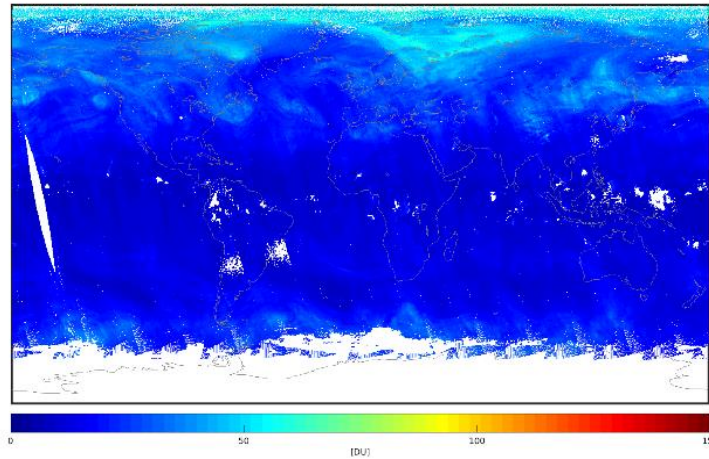
Daily global maps: subcolumns

Subcolumn ozone for OFFL products, April 29, 2022

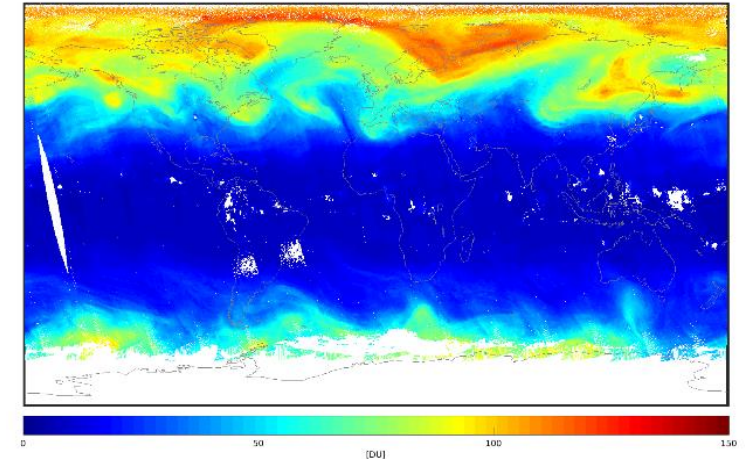
0-6 km



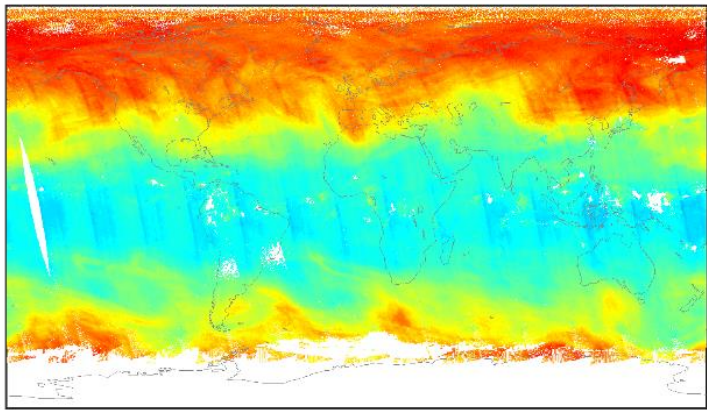
6-12 km



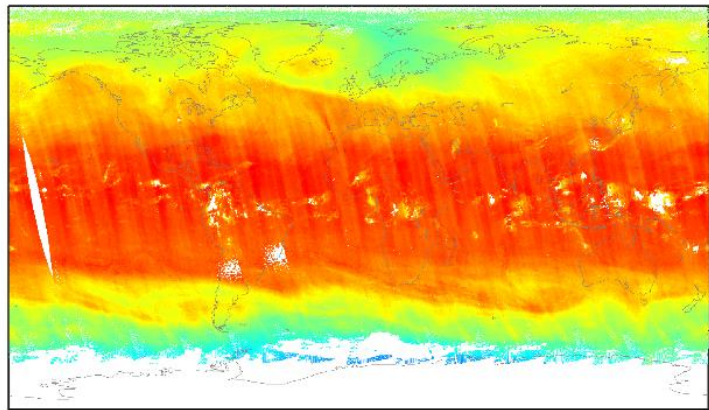
12-18 km



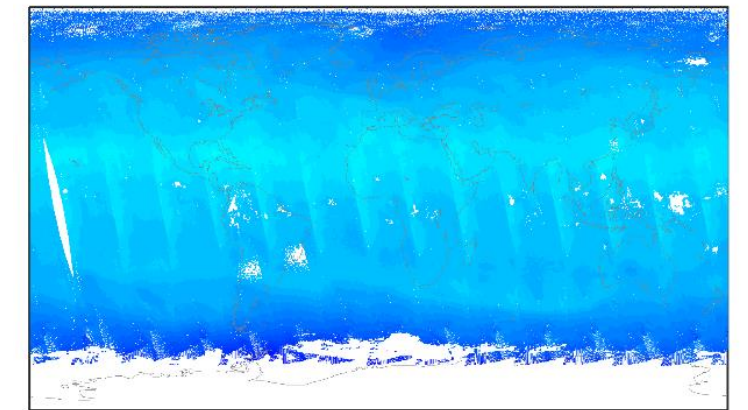
18-24 km









24-32 km

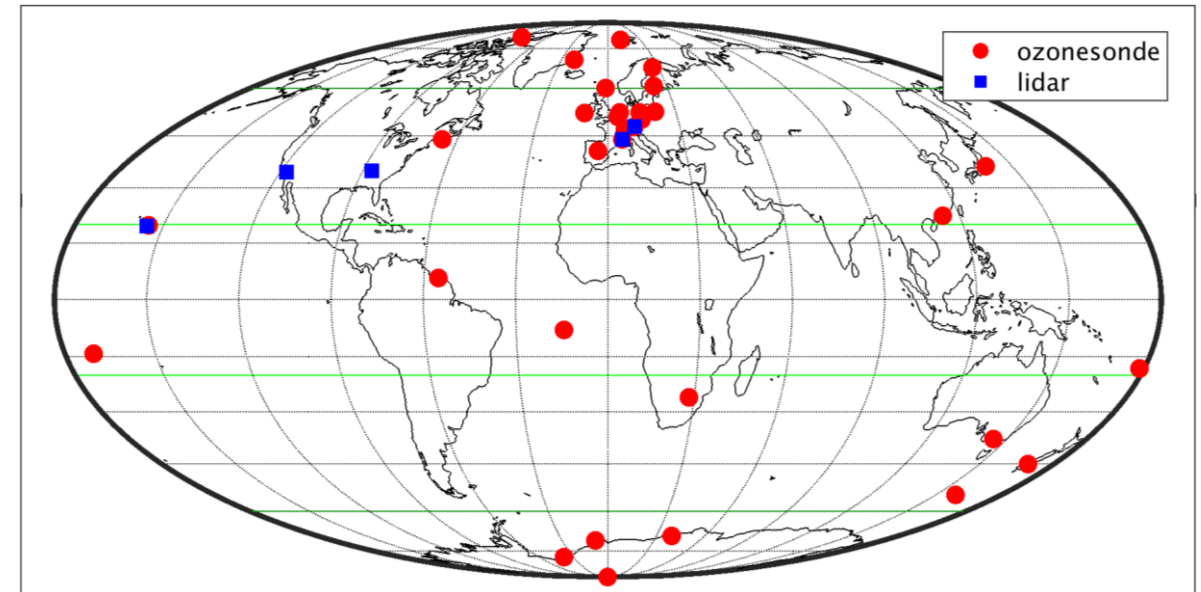


32 km - TOA



Ground-based validation: data & settings

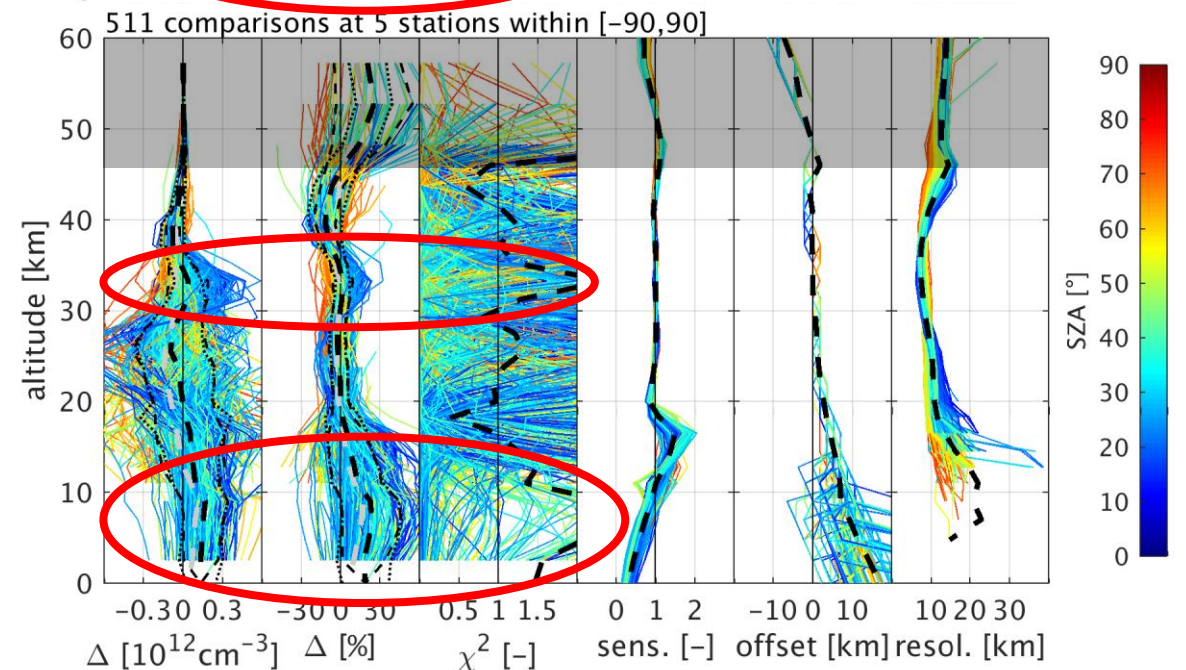
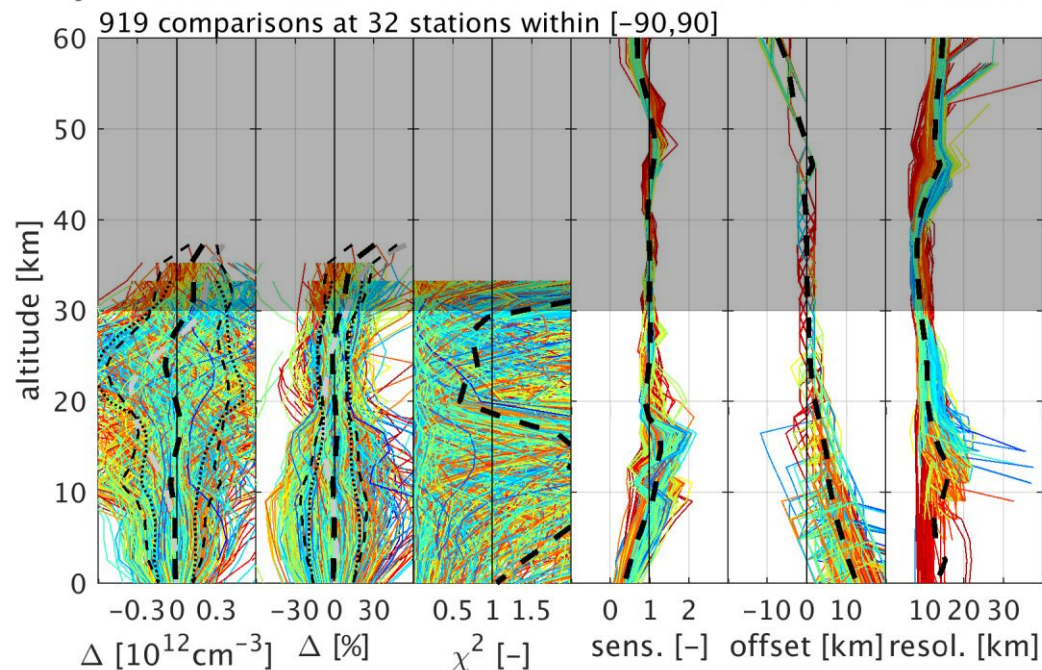
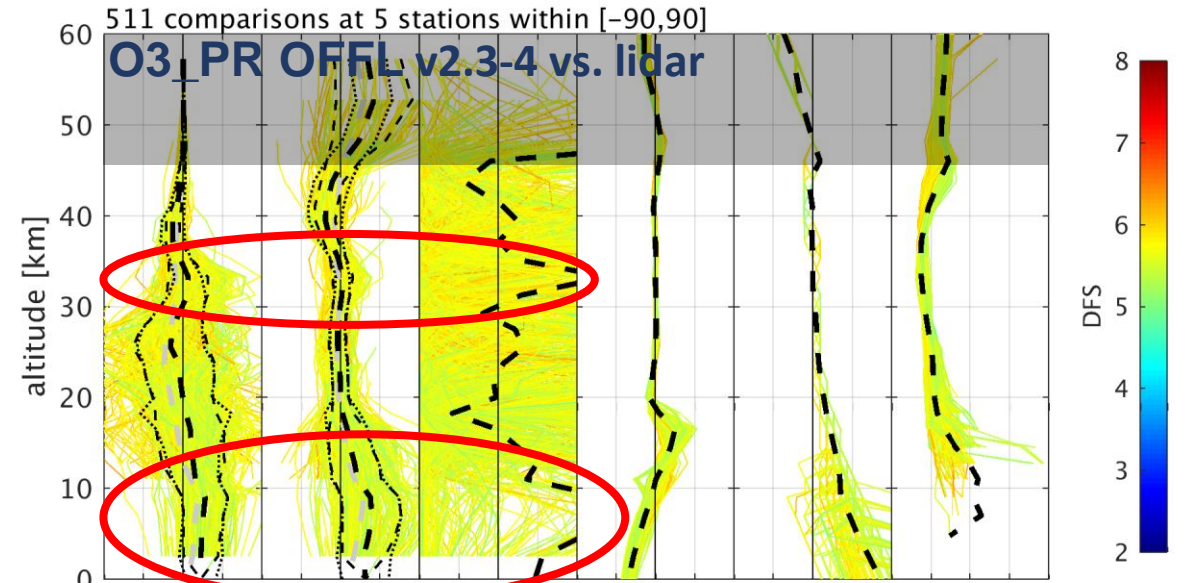
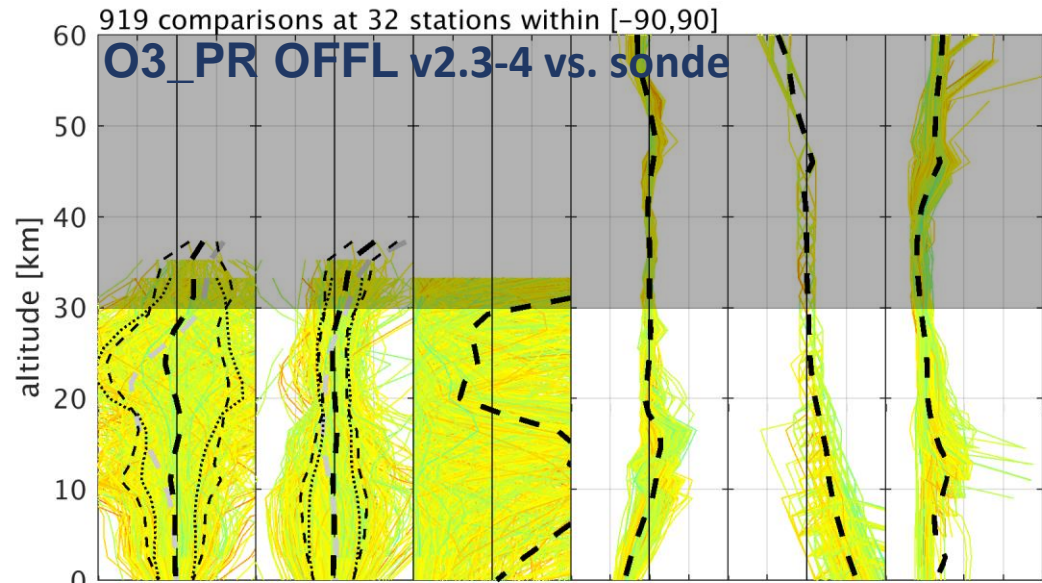
- OFFL (and NRTI) O3_PR for qa_value > 0.5
- Validation data (FRM) through EVDC 
 - NDACC/SHADOZ/WOUDC networks + MATCH campaign ozonesonde   
 - NDACC/TOLNET tropospheric and stratospheric lidar  
- Co-location
 - same day (± 12 h)
 - overpass pixel (AVS: “point-in-area”)
- 1400+ co-located data pairs by 2022/09
 - 32 ozonesonde stations
 - 5 lidar stations
- Mass-conserved regridding and averaging kernel smoothing of FRM data (Keppens et al., 2019)



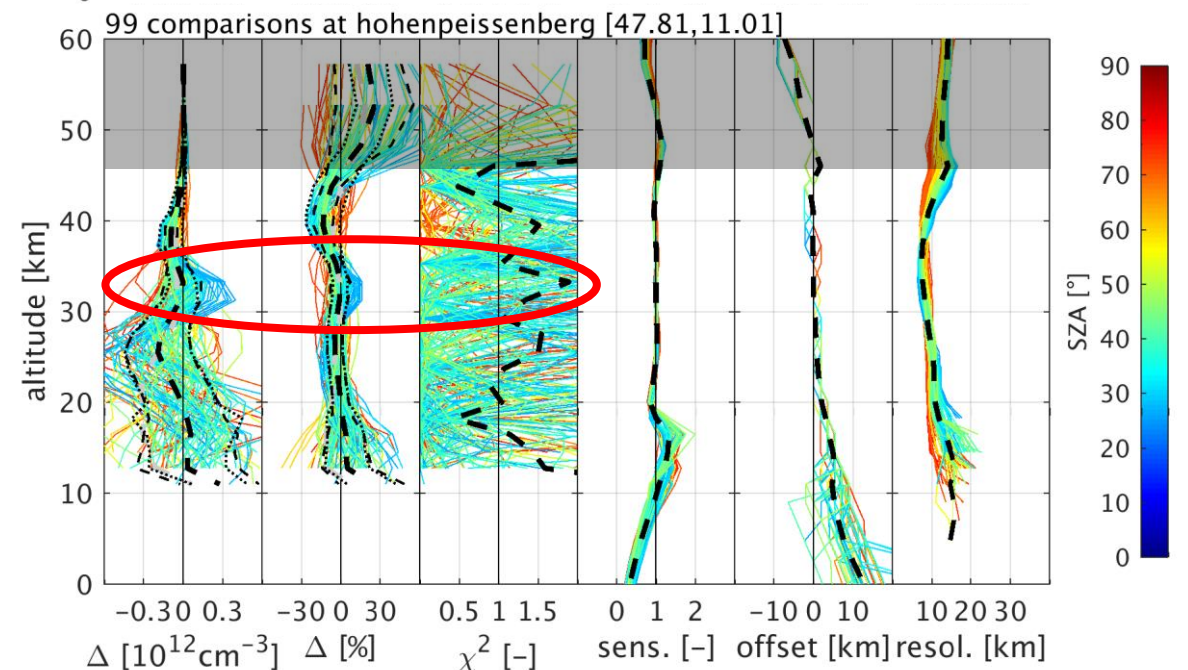
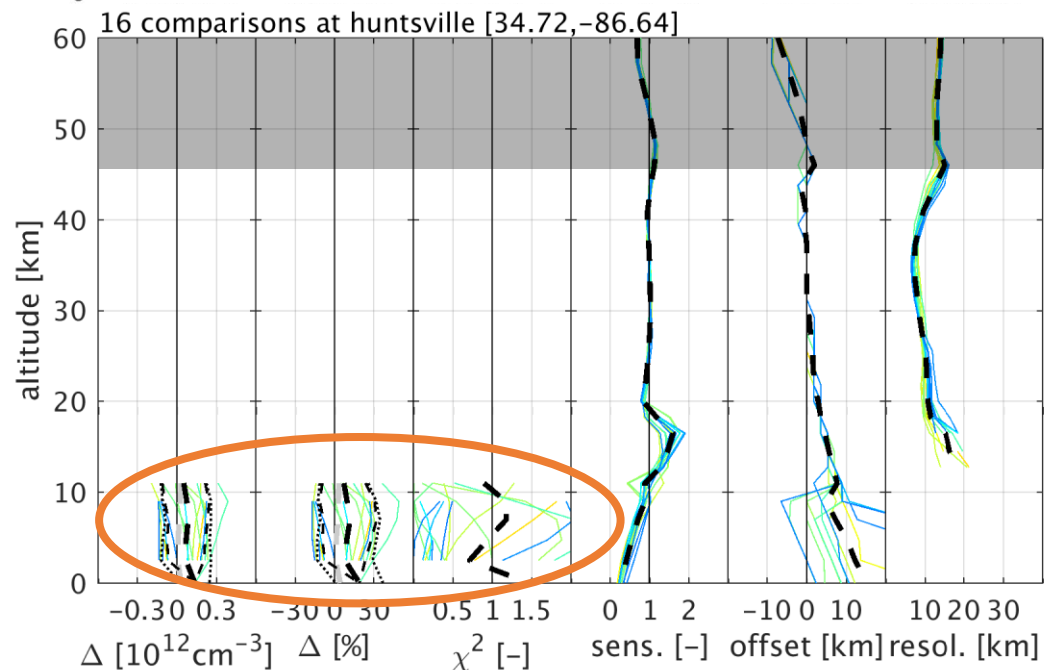
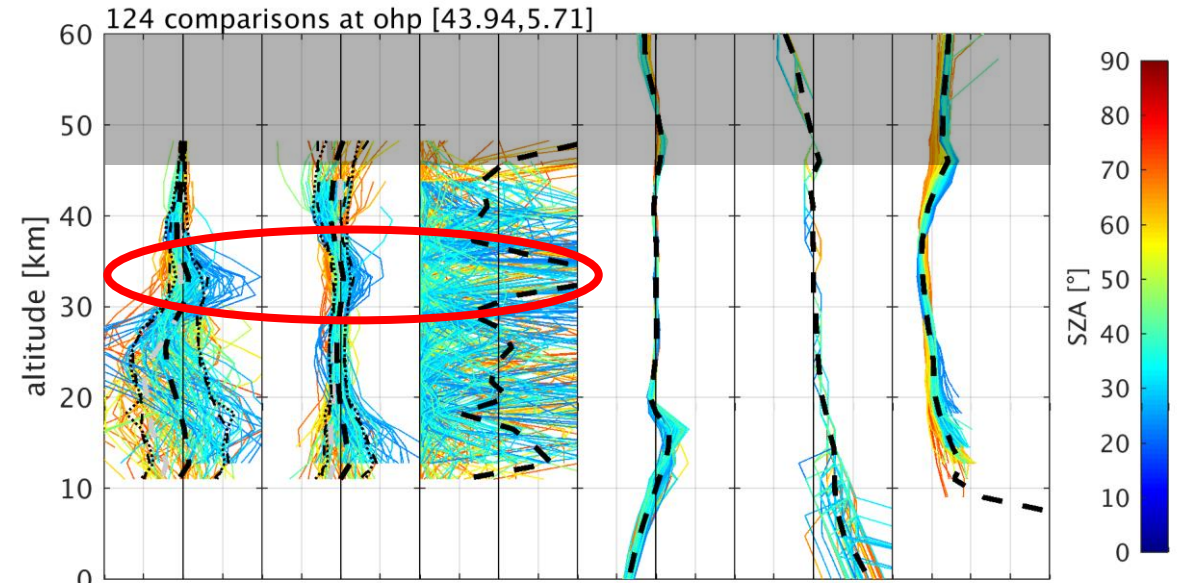
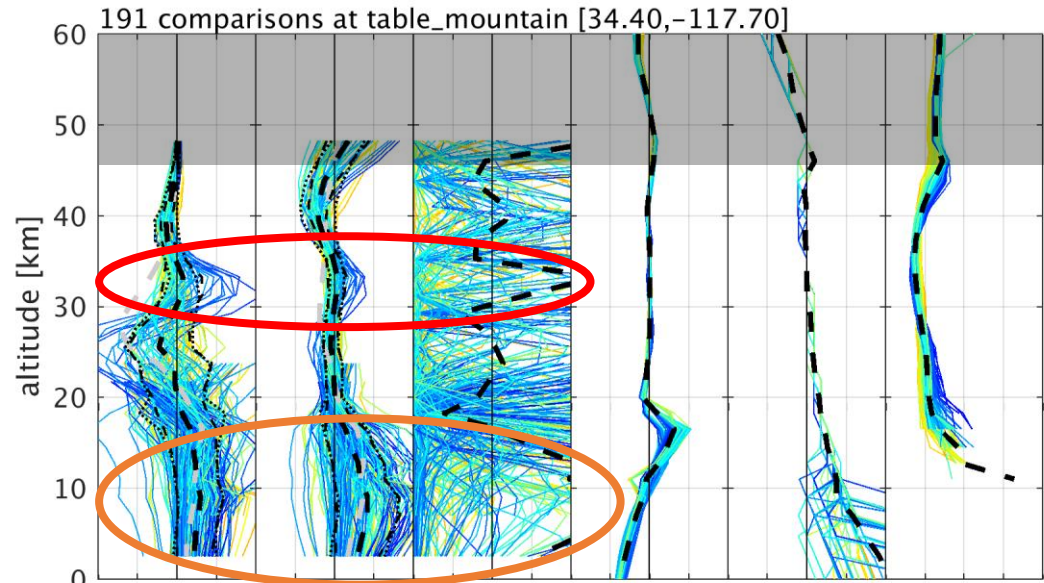
Comparisons and information content

- Comparison statistics
 - absolute & relative differences
 - χ^2 -test after AK smoothing: square measure of the difference w.r.t. combined ex-ante uncertainties
 - correlations for subcolumns
- Information content
 - vertical sensitivity: AK row sums
 - retrieval offset: AK peak altitude versus nominal altitude
 - effective vertical resolution: AK FWHM
- All with respect to influence quantities
 - latitude, time, SZA, VZA, cloud fraction, surface albedo...

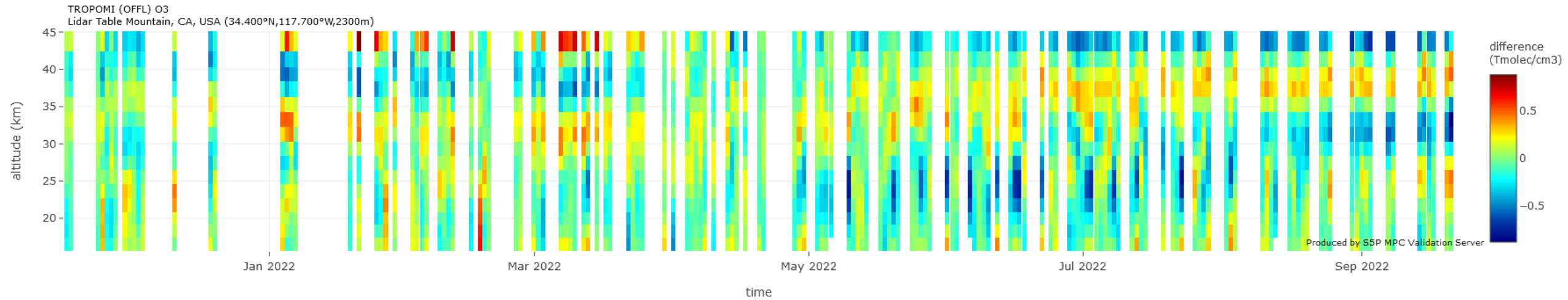
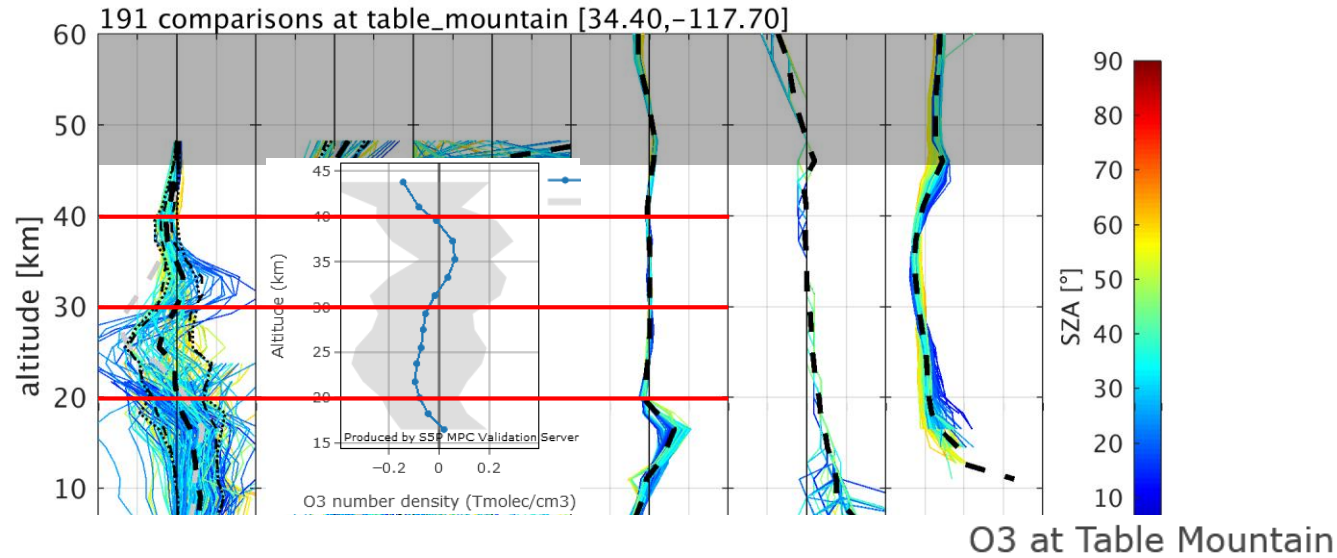
Comparisons and information content: global



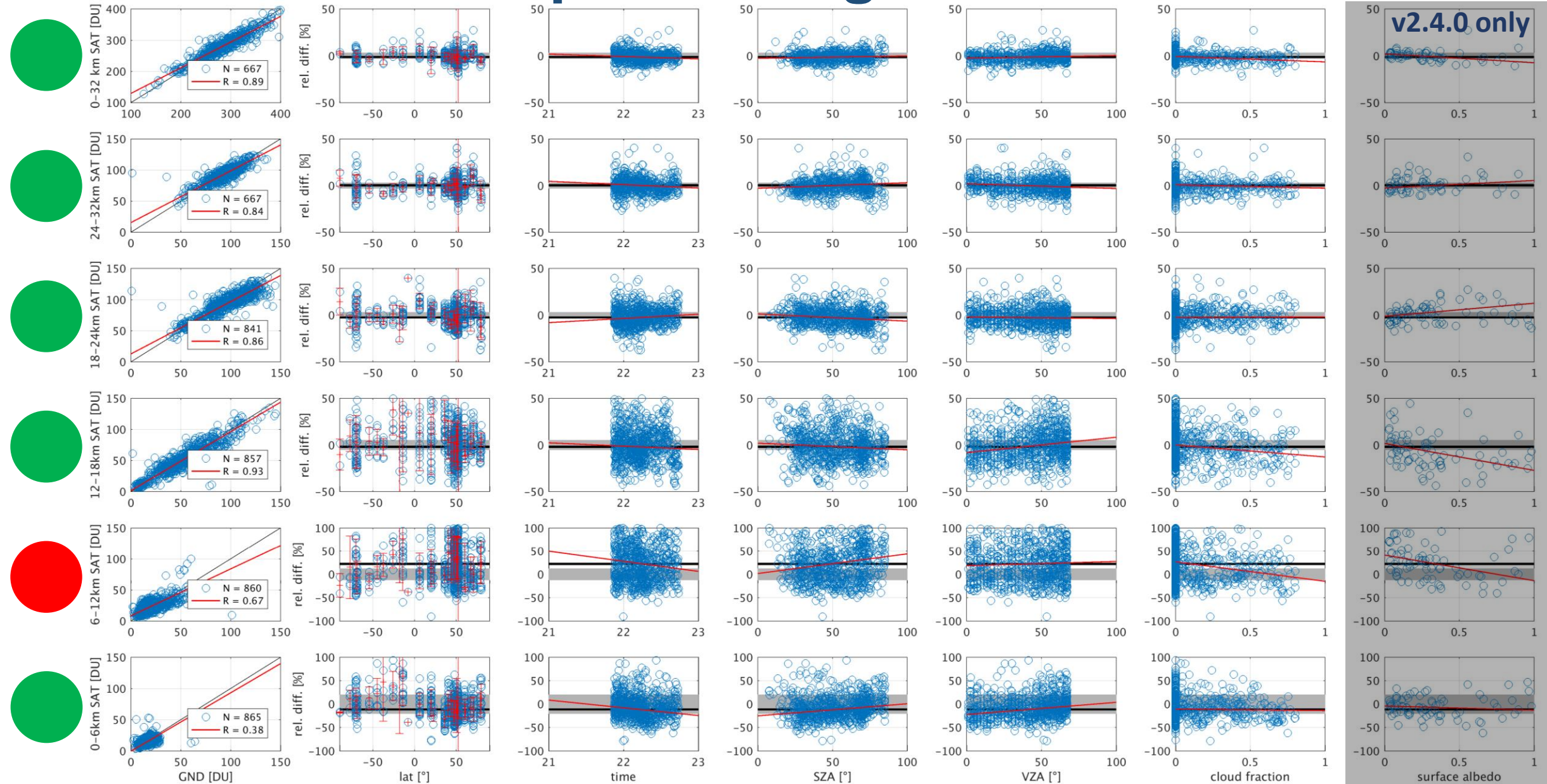
Comparisons and information content: lidar



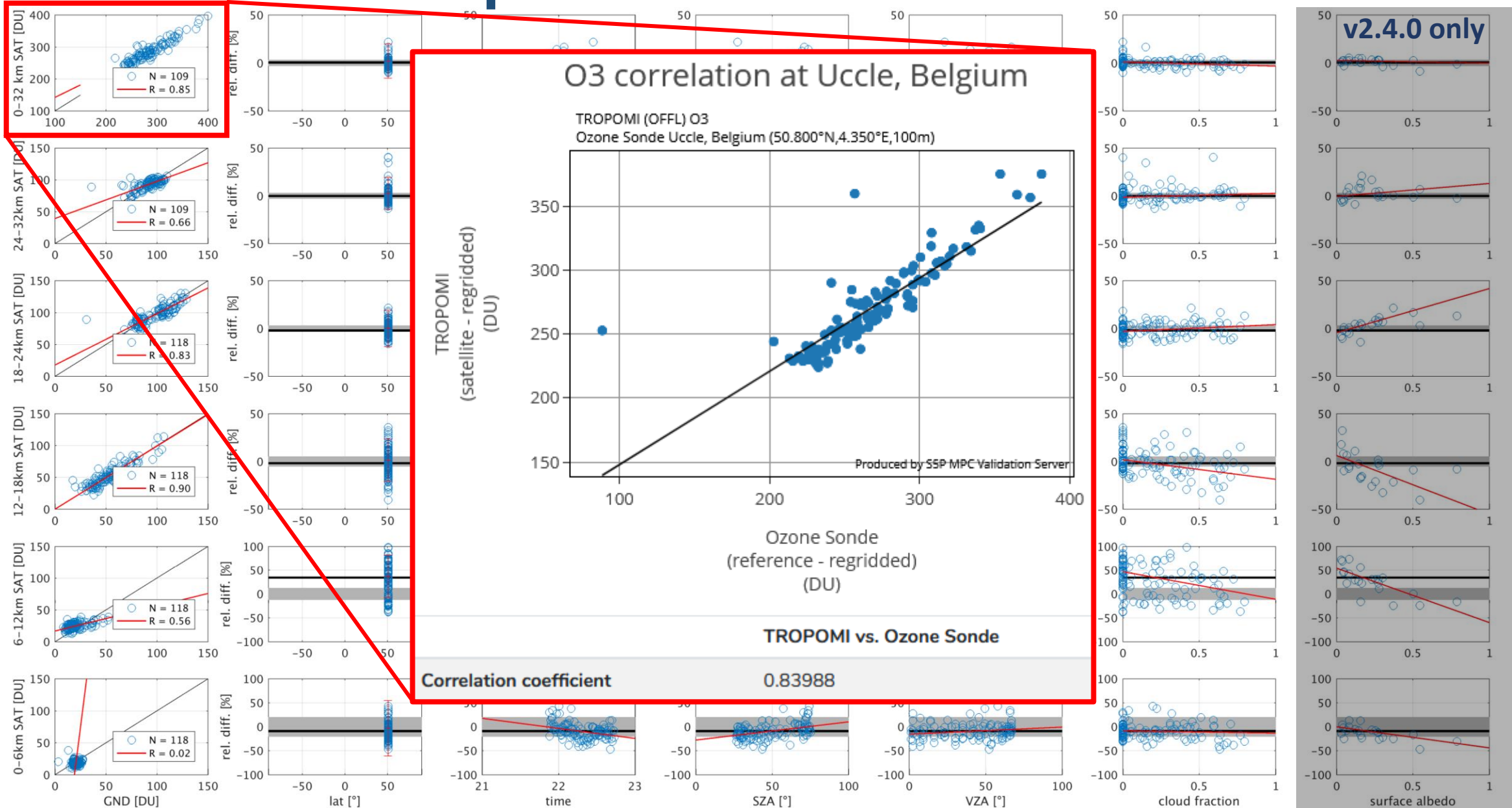
Comparisons and information content: lidar



Subcolumn comparisons: global sonde stations



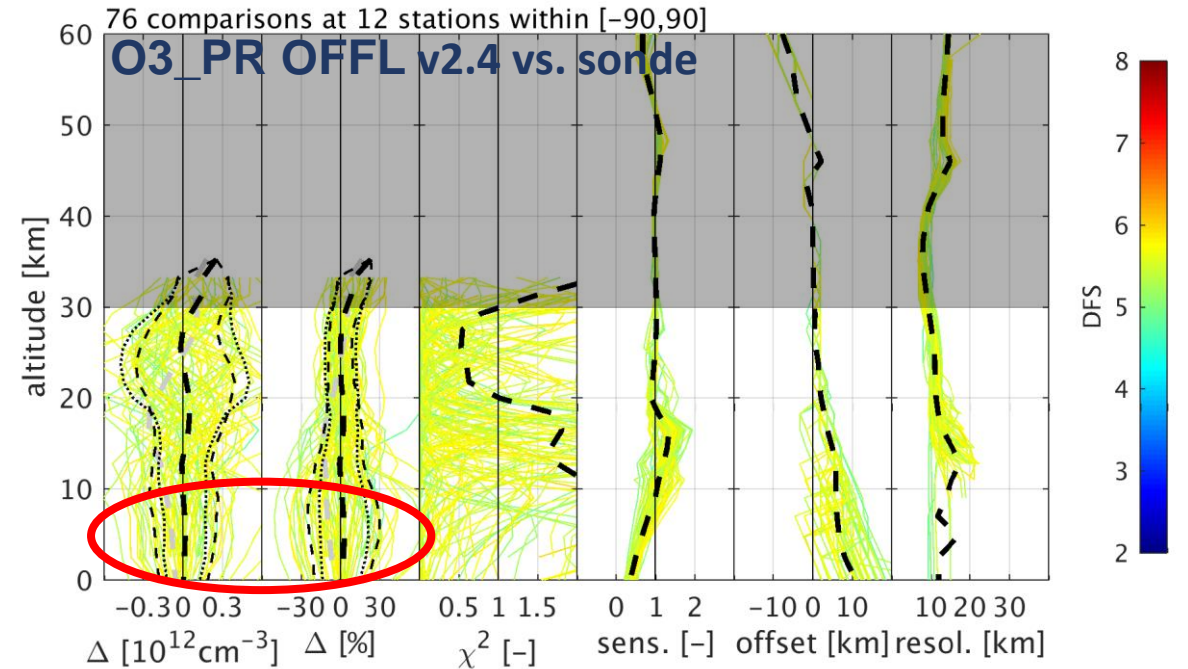
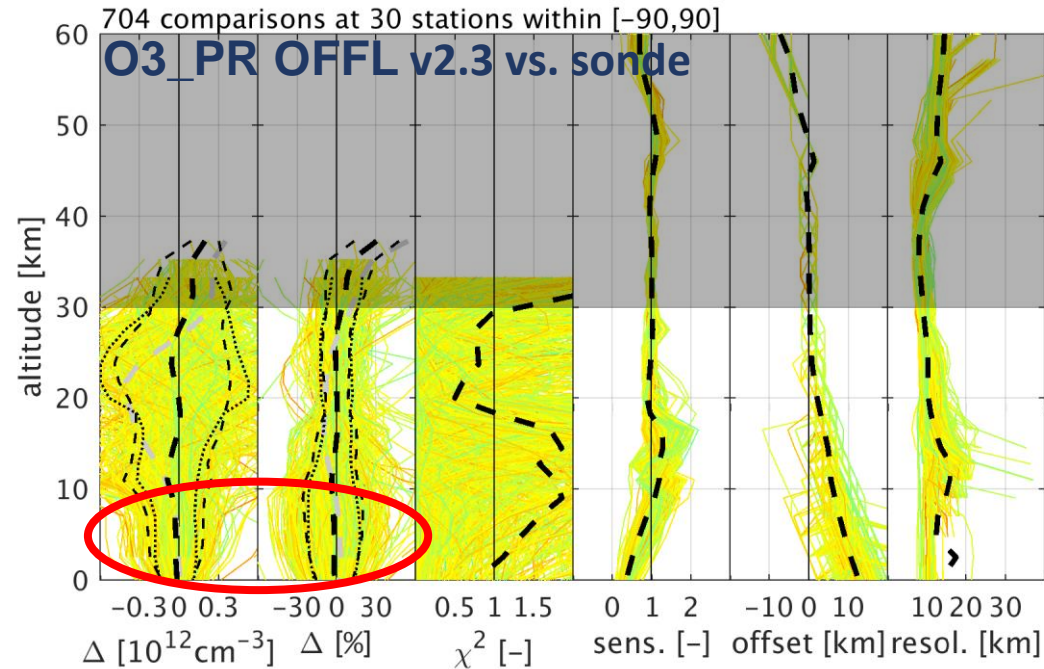
Subcolumn comparisons: sonde at Uccle



Validation results summary

- DFS: consistently close to 6 pieces of independent information
- 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
- Bias below 10 %, vertical oscillations in stratosphere, especially for low SZA
- Dispersion ~20 % below TP, 5-10 % above
- Ex-ante uncertainty underestimated around TP and below, and around 35 km for low SZA
- Integrated profile consistent with total column retrieval and integrated ozonesondes
- High correlation with ozonesonde data in 12-32 km sub-columns
- Slight striping along orbit (TBC for updated soft-calibration)
- Reduced retrieval quality for high/low SZA and surface albedo, especially around Antarctic
- No significant effect of L1B and L2 version updates (July 2022) on product quality (TBC, increased tropospheric ozone column observed by KNMI)



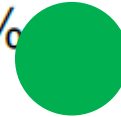
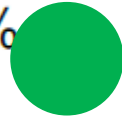
Validation results summary



- No significant effect of L1B and L2 version updates (July 2022) on product quality (TBC, increased tropospheric ozone column observed by KNMI)


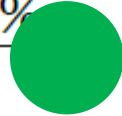

Compliance with requirements

- Science Requirements Document (2008) and ATBD (2021):

Sub column	PBL ¹⁾	0 - 6 km	6-12 km	12-18 km	18-50 km
Required accuracy	≤ 60 %	≤ 20 % 	≤ 12 % 	≤ 5 % 	≤ 3 % 

¹⁾ In practice the pressure at the top of the planetary boundary layer is not known and results for this sub column cannot be provided. Simulation studies can be used to estimate the accuracy for the PBL.

- Scientific Validation Implementation plan (2016) / Cal-Val plan (2017):

Parameter	Data Product	Vertical Resolution	Accuracy	Precision
Ozone	Ozone Profile	6 km 	10-30% 	10% 

Poster 15 (Verhoelst et al.): Validation of Sentinel-5P operational ozone data products: Status, advances and remaining challenges