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Sentinel-5P TROPOMI tropospheric ozone: scientific retrieval upgrades and comparison to operational data

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IUP

SHADOZ

0. Input data and models:

S5P/TROPOMI Level 2 input data: OFFL GODFIT ozone, ghost column, OCRA/ROCINN cloud pressure, height, fraction (known..)

CHORA-CCD and CHOVA-CS retrieval models

NASA/GSFC SHADOZ ozone sonde profiles for validation

GODFIT: / OCRA: / ROCINN IUP processor (Cloud Height and Ozone Variation Algorithm)

S5P/TROPOMI input data: CF, TCO, and SD1σ

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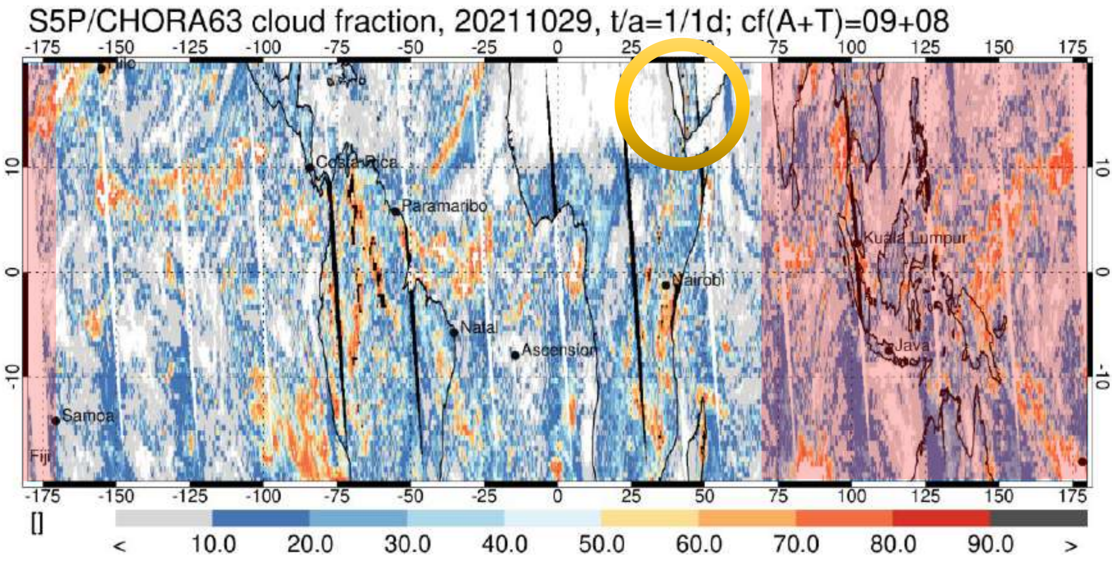
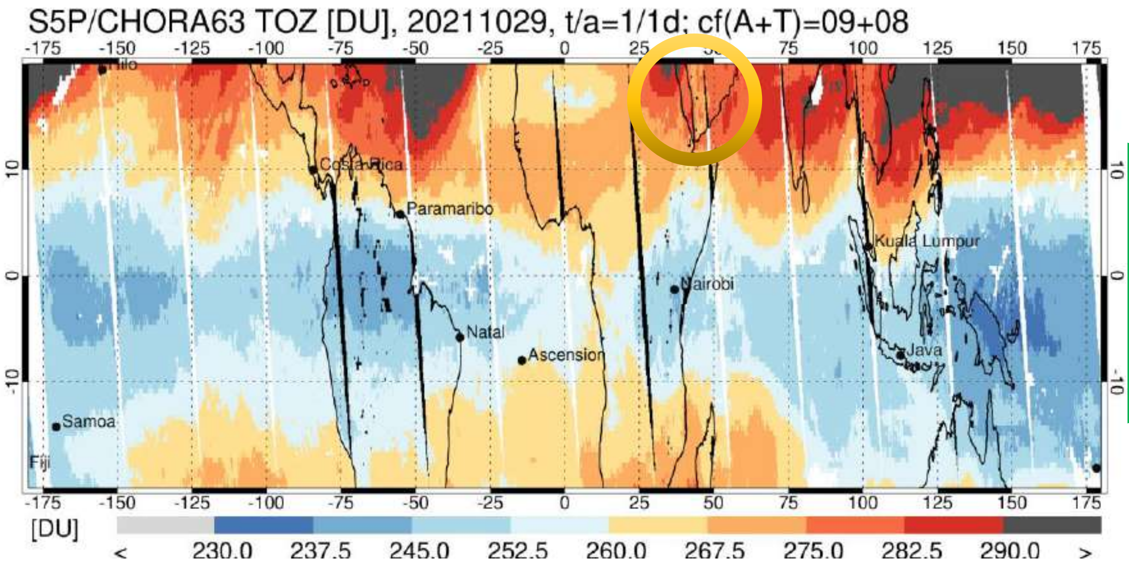
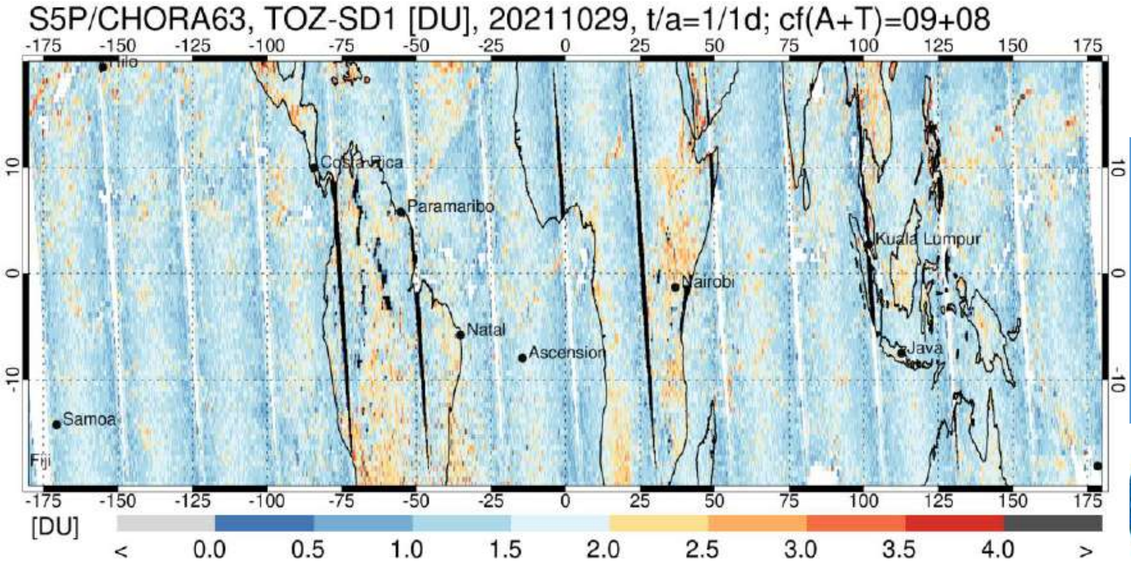




Cloud fraction (CF) gridded map shows that the tropics are **mainly cloud free** (**CF<20%**).

Total ozone (TCO) binned for **CF<80%.** Meridional ozone variations in the tropics are about 50 DU.

TCO **standard deviation** (1σ) shows orbital structures with larger values in the center and reduced SD especially in the eastern part of an orbit. Note: Less measurements per grid box towards the edges.



IUP

CHOVA V6.6: Cloud Height and Ozone Variation Analysis

06.10.22

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Tropical Tropospheric Ozone (TTO) volume mixing ratio retrieval (CSA) using collocated cloud top pressure and above-cloud column ozone measurements.

Robust Theil-Sen regression reduces influence of outliers and heteroscedacity in total ozone and cloud parameters.

Quality value module using total ozone, cloud top pressure, and regression parameters to exclude bad data.

Data: S5P/TROPOMI **total ozone** (GODFIT) and **cloud height** (CRB; CRA/ROCINN)

Processor versions: OFFL/RPRO ≤ V02.04.01.

Sampling parameters:

Temporal: **daily**

Boundaries: **20°N/S**

Grid size: **3°x3°**

Stepwidth: **2°Lat/Lon**

Atmospheric boundaries:

CF > 0.95

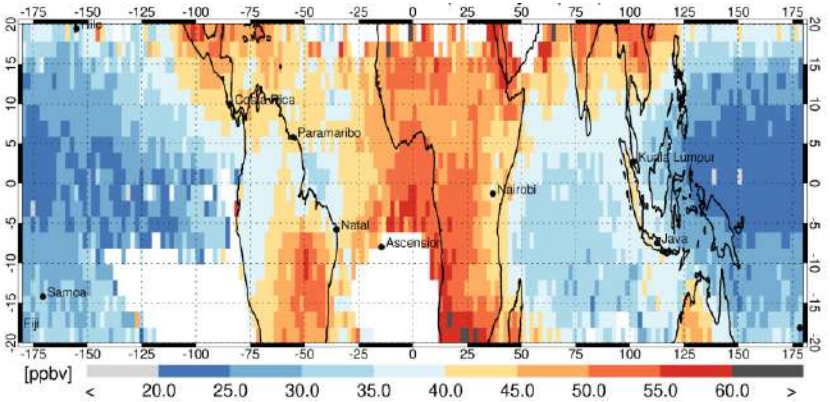
CH ~ [5-13 km]

Mn(CP) < 320 hPa

Mx(CP) < 550 hPa

□CP > 100 hPa

Based on: *Cloud slicing technique (Ziemke et al., JGR 106D9, 2001).*



2019 annual mean CHOVA TTO [ppbv] (Europe centered view).

CHORA(PS) V6.4/7.0: Cloud Height Ozone Reference Algorithm

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CHORA/CCD retrieves **Tropical Tropospheric Column Ozone (TTCO) by** substracting „stratospheric“ mean ozone from total ozone.

The Above Cloud Column Ozone (ACCO) calculated in the **Pacific sector (PS)** is used to represent the stratospheric column.

ACCO for reference pressure level **270 hPa**: (**6.4**) CHOVA monthly mean ozone / (**7.0**) direct calculation via Theil-Sen regression.

Based on: *Convective cloud differential technique (Ziemke et al., JGR 103D17, 1998)*.

Data: S5P/TROPOMI **total ozone** (GODFIT, WFDOAS) and **cloud heights** (CRB; OCRA/ROCINN).

Processor versions: OFFL/RPRO ≤ V02.04.01.

Sampling parameters:

Temporal: **daily**.

Boundaries: **20°N/S**

ACCO box: [70E,170W]

ACCO step/size: **0.5°/1°**

TOZ grid: **0.5°x0.25°**

Atmospheric boundaries:

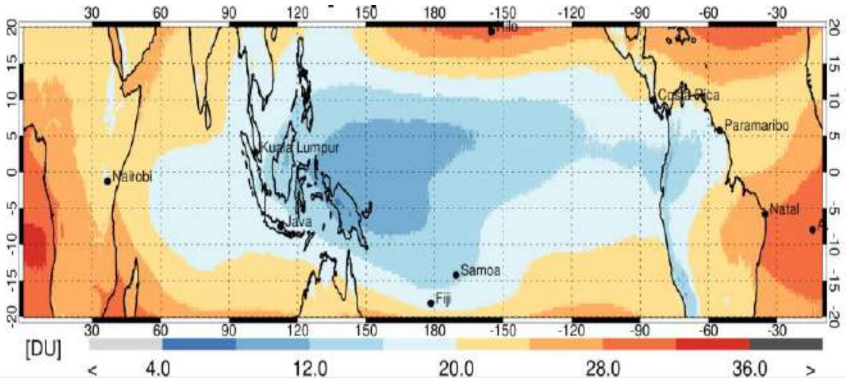
- **Stratosphere** (ACCO):

CF ≥ **0.8**

CP < 350 hPa

CP_{ref} = 270 hPa

- **Total** (TOZ): CF ≤ **0.8**



2018-2021 CHORA-PS TTCO [DU] (Pacific centered view).

NASA/GSFC SHADOZ ozone sonde profiles

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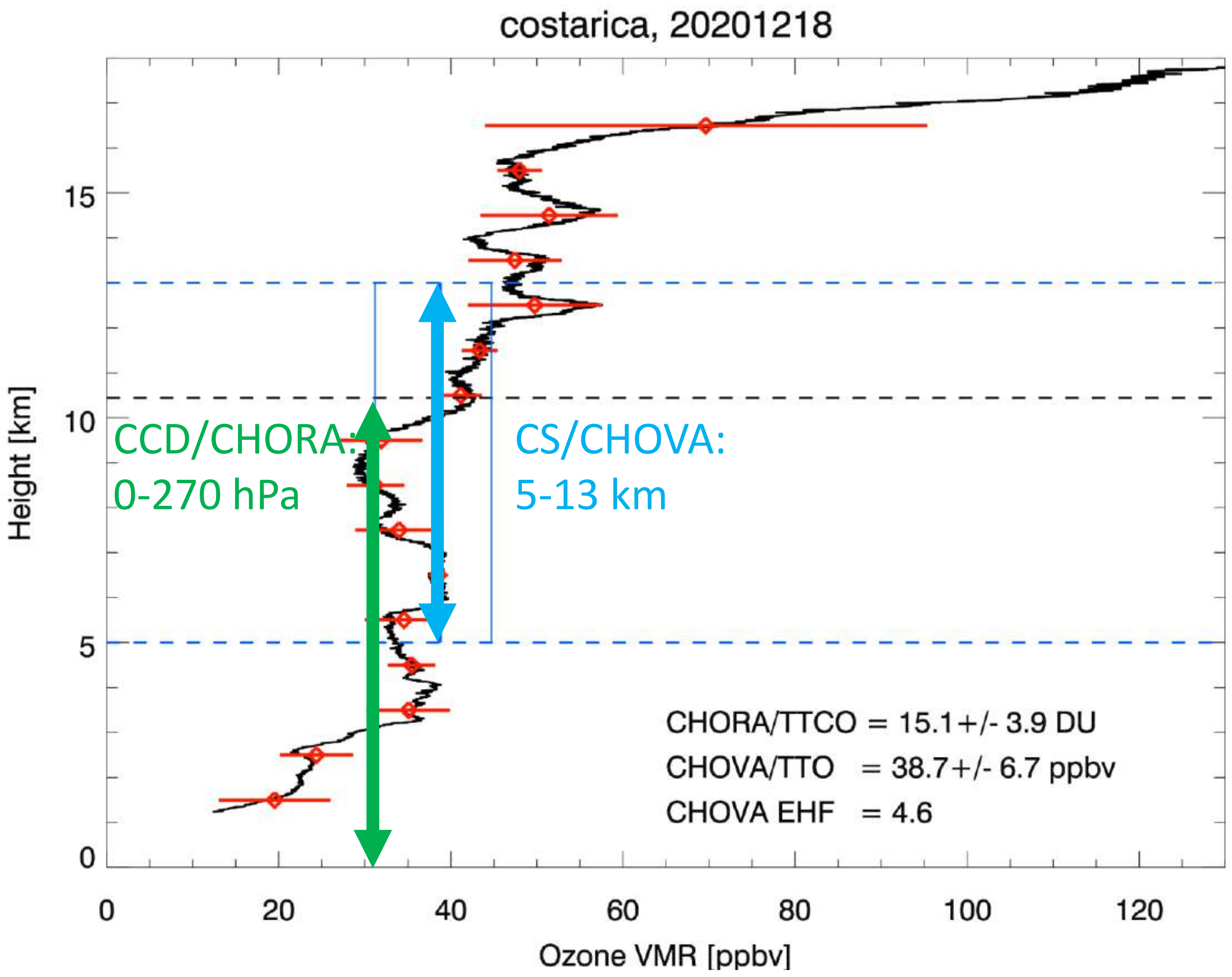

Black line: Ozone sonde volume mixing ratios [ppbv] of Costa Rica (2020/12/18). Red diamonds and line: Average VMR and standard deviation SD(1σ) at 1km resolution.

Calculation of subcolumn ozone up to **270 hPa** reference height [black dashed line] for CHORA TTCO validation. Conversion of VMRs to number densities to calculate DU and SD1.

Calculation of median VMR and IP68 for the 5 to 13 km height range [blue dashed lines] for CHOVA TTO validation.

Data from: https://tropo.gsfc.nasa.gov/shadoz/index.html

1. Cloud Slicing: CHOVA V6.6

Data coverage and seasonal maps

Comparisons with NASA/GSFC SHADOZ ozone sondes

(Towards the operational processor version: IDL -> PYTHON)

CHOVA=Cloud Height and Ozone Variation Algorithm: IUP processor

S5P CHOVA 6.4 TTO seasonal means 2020

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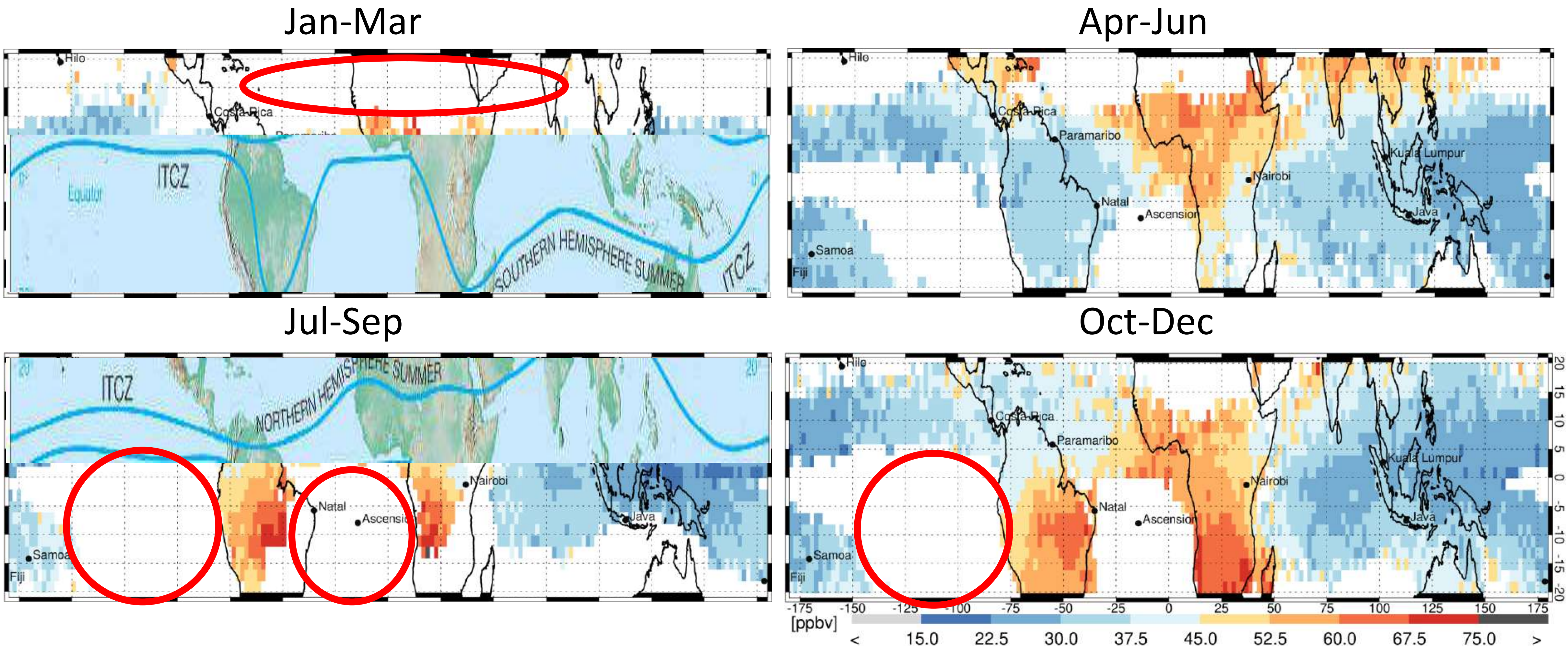

: large areas of cloud top height < 5 km and/or cloud free areas

CHOVA validation with SHADOZ ozone sondes: e.g. Kuala Lumpur

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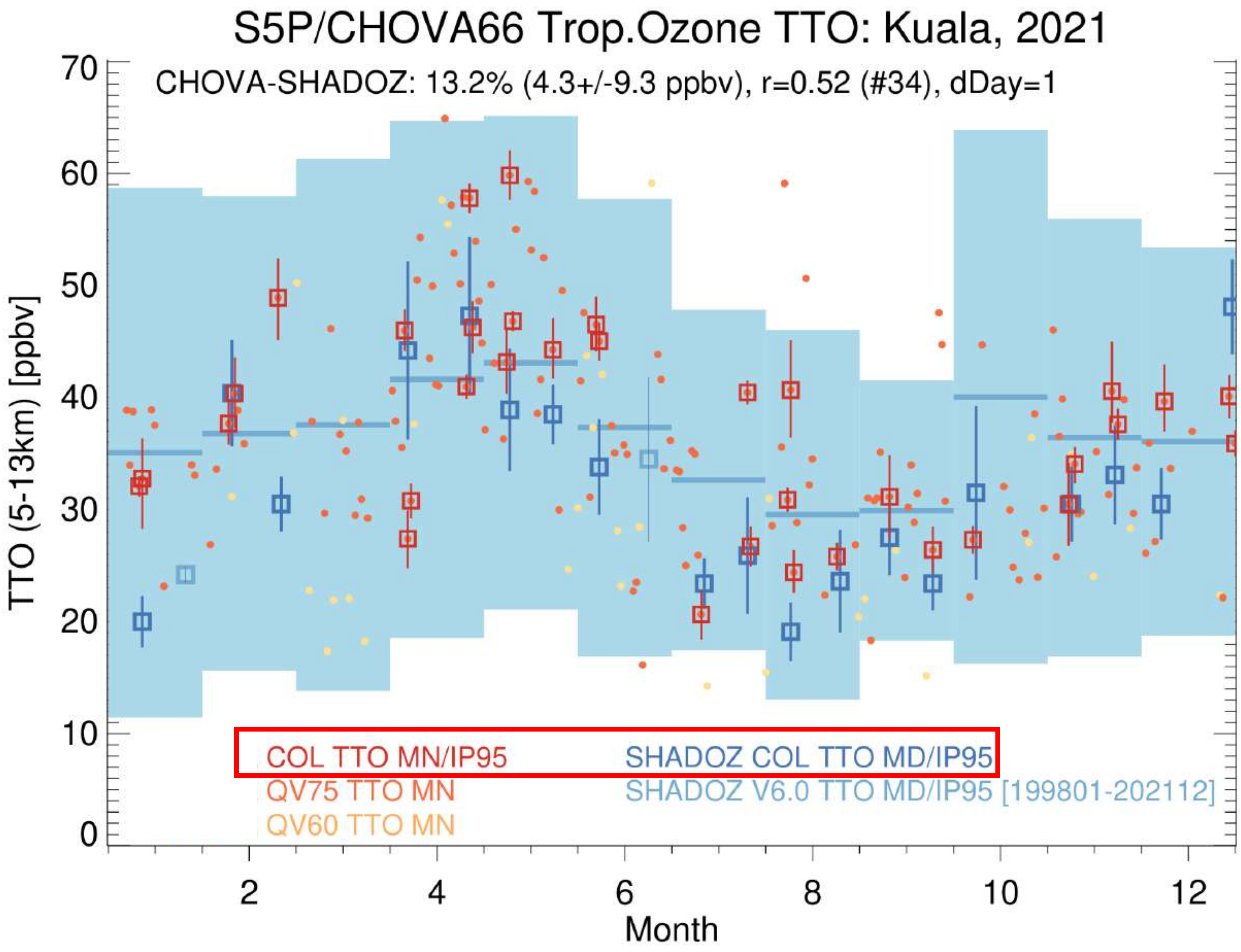
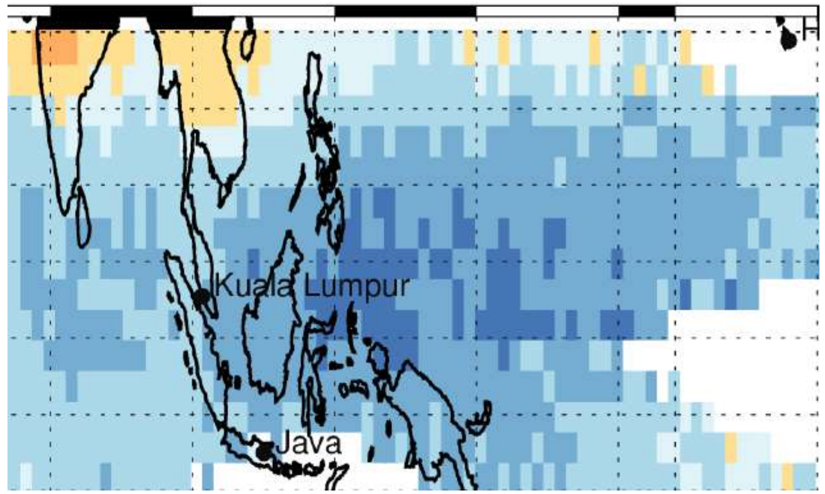




CHOVA VMRs (and 95% IP) follow the annual cycle with 60 ppbv in Spring and 30 ppbv in Autumn.

CHOVA overestimates collocated SHADOZ median VMRs by 13% with Pearson r of 0.52 and a dispersion of 9.3 pbbv.

CHOVA validation with SHADOZ ozone sondes: general view

CHOVA 6.6 TTO and ***median*** ozone sonde VMR [5-13km] (ppbv) with QV>60

S5P OFFL/RPRO 01.01.07-02.03.00 (May 2018 – May 2022)

7 NASA/GSFC SHADOZ V6.0 sonde sites: Costa Rica, Fiji, Kuala Lumpur, Nairobi, Natal, Paramaribo, Samoa

Collocated pairs for **0 *day*** difference: **130**

TTO: CHOVA-SONDE	Bias-Median	IP68/2
Difference [ppbv]	0.1	11
RD [%]	**0.4**	**32**
Low VMR RD [%]	13	34
High VMR RD [%]	-11	24

Bias (Req. 25%, ~5-15 ppbv):

median bias (0.4%), negative bias (-11%) for high VMR and vice versa (13%)

Spread (Req. 25%):

IP68/2 dispersion (32%)

Correlation (Pearson) 0.45

2. Convective cloud differential: CHORA-PS V6.4/7.0

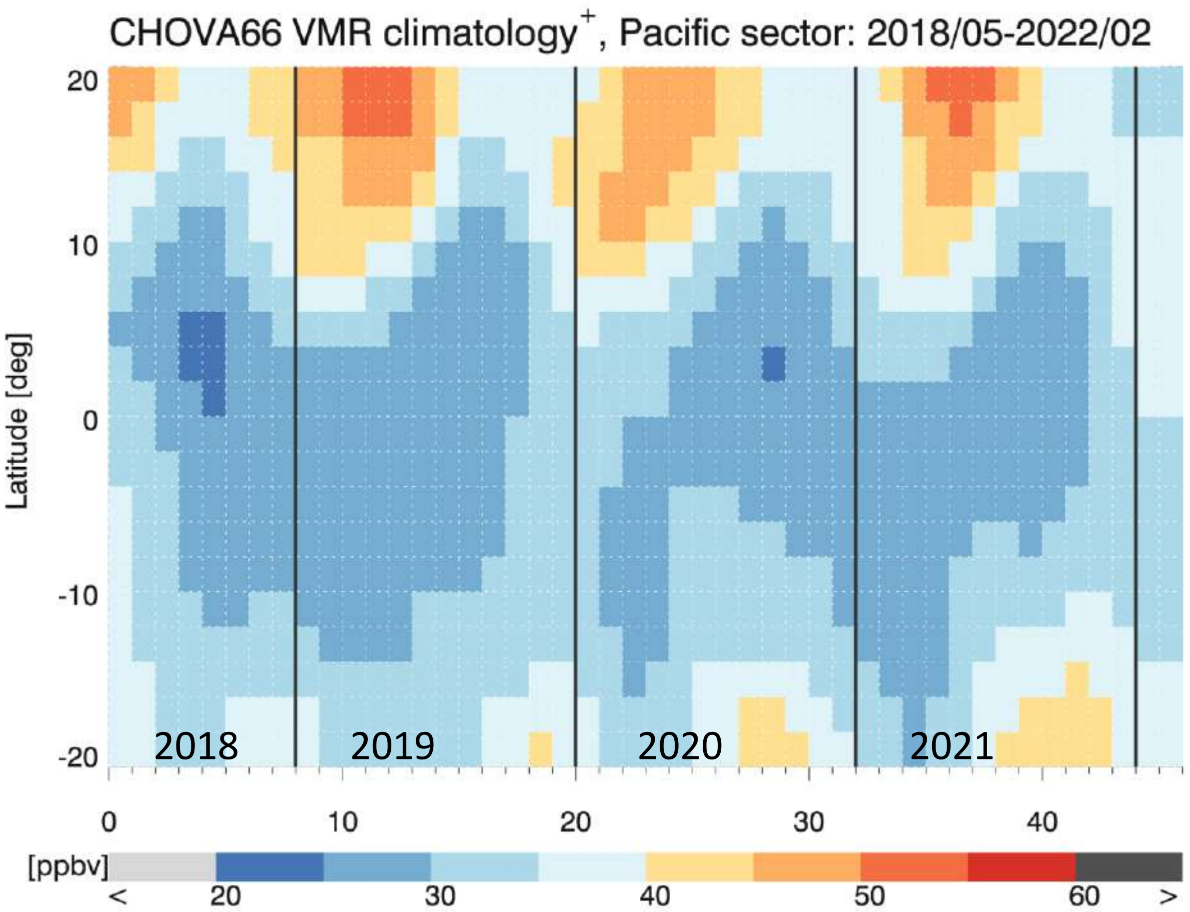
Use of CHOVA cloud height correction (V6.4) and independent correction (V7.0)

ACCO upgrading

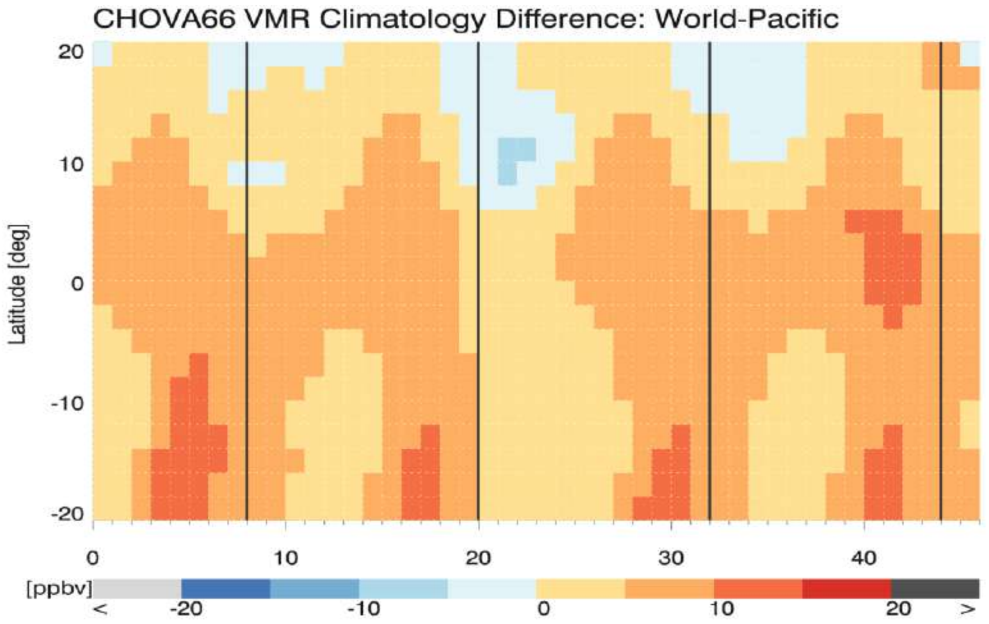
Comparisons with NASA/GSFC SHADOZ ozone sondes

CHORA=Cloud Height and Ozone Reference Algorithm; PS=pacific sector, IUP processor

Step 1: CS ozone VMRs for CCD cloud height correction in CHORA V6.4



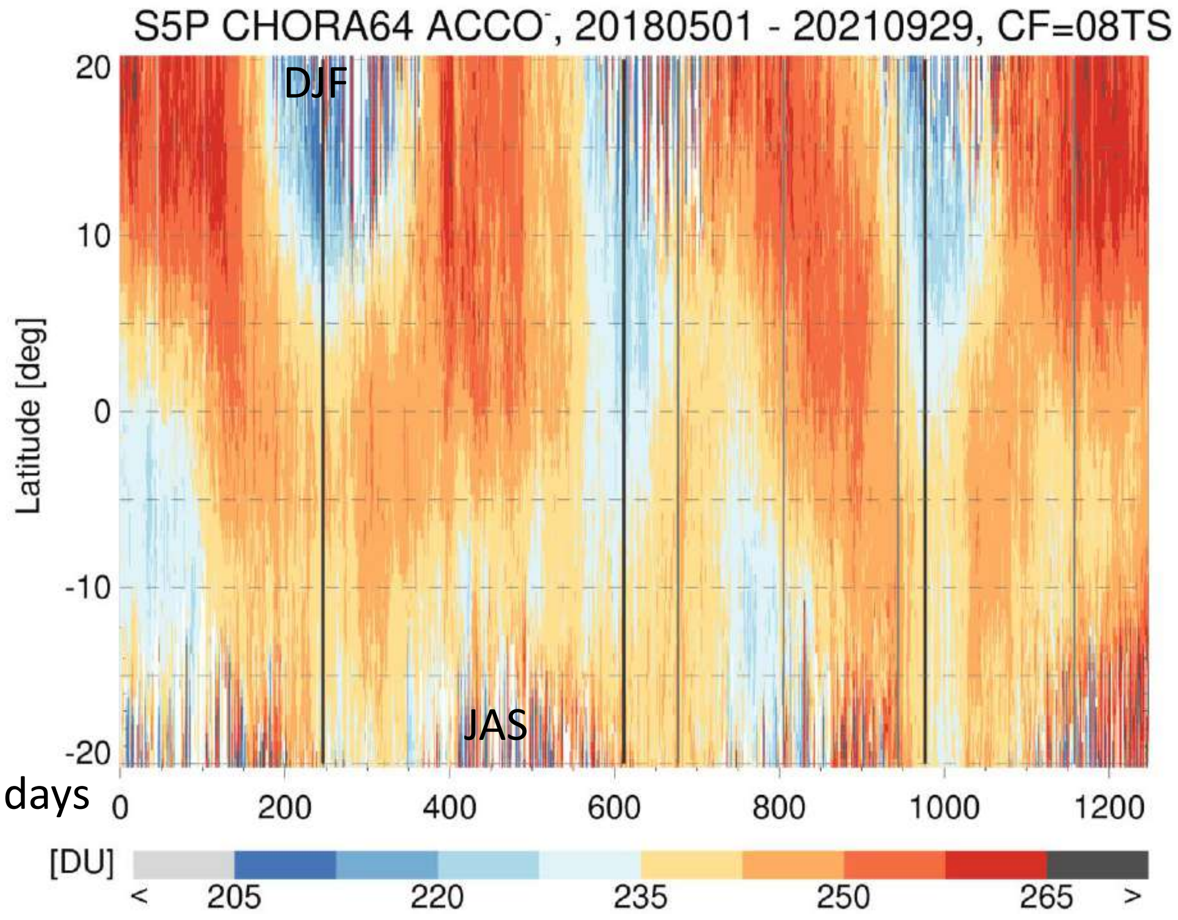
CHOVA66 TTO zonal monthly means [ppbv] of the Pacific sector [70E-170E] on a 2° latitude grid for May 2018 – February 2022.

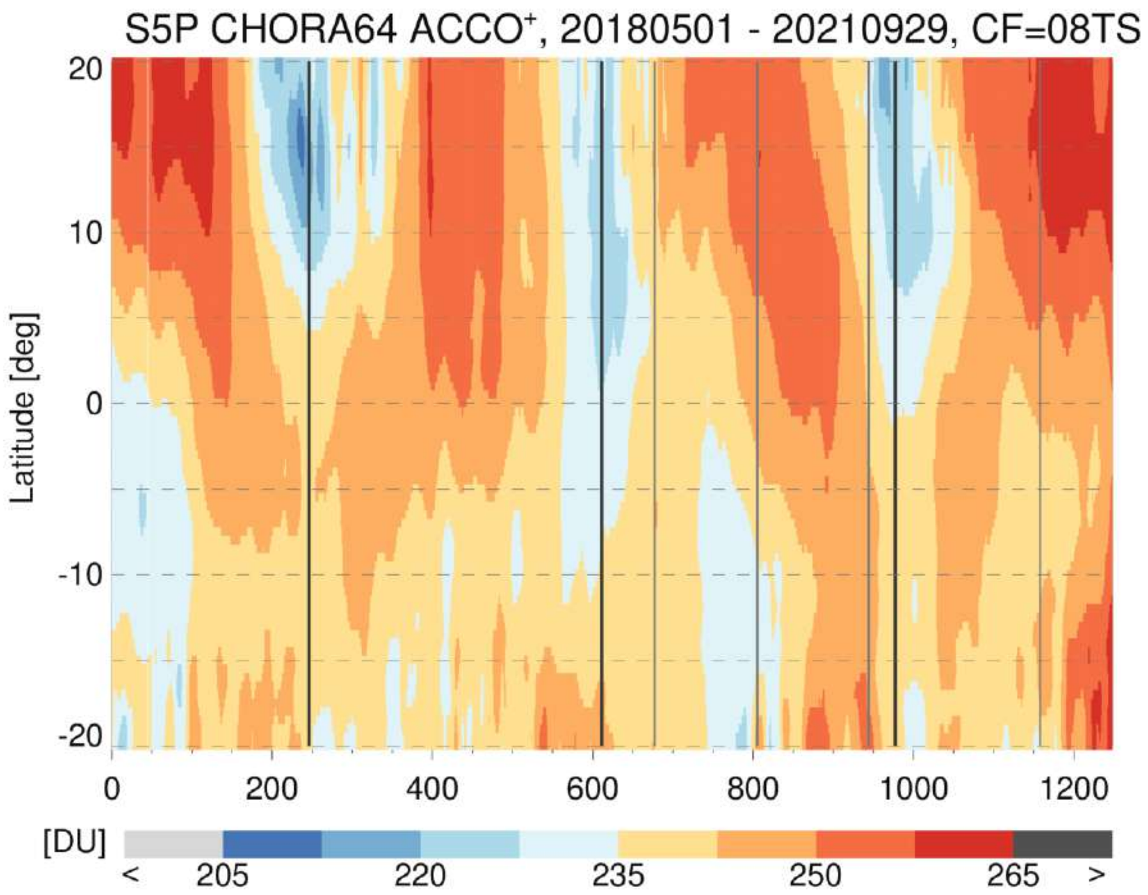


TTO difference of World vs Pacific values. Differences are mostly within 0-10 ppbv, but can be up to 15 ppbv in southern Autumn.

Lower clouds (higher pressure) than the reference pressure have a **negative CC**, a smaller *ACCO* and a **larger TTCO**. Underestimating the cloud height (typical for TROPOMI) adds a positive bias to TTCO. If CC is not adjusted to the Pacific sector (where zonal mean climatologies are too high), it **enhances the high bias**.

Step2: Time-latitude ACCO post-processing in V6.4 and V7.0





CHORA V6.4 ACCO based on Theil-Sen regression instead of using climatology for the height correction. Data gaps occur due to missing data and seasonal cloud height/fraction changes. High frequency scatter towards the extra-tropics.

ACCO 2-d field upgraded from raw data. Gaps are filled and short term scatter/noise in latitude/time direction reduced. The large areas of missing data (DJF) are less accurate and can be excluded via quality flag.

CHORA V6.4 TTCO seasonal mean 2021

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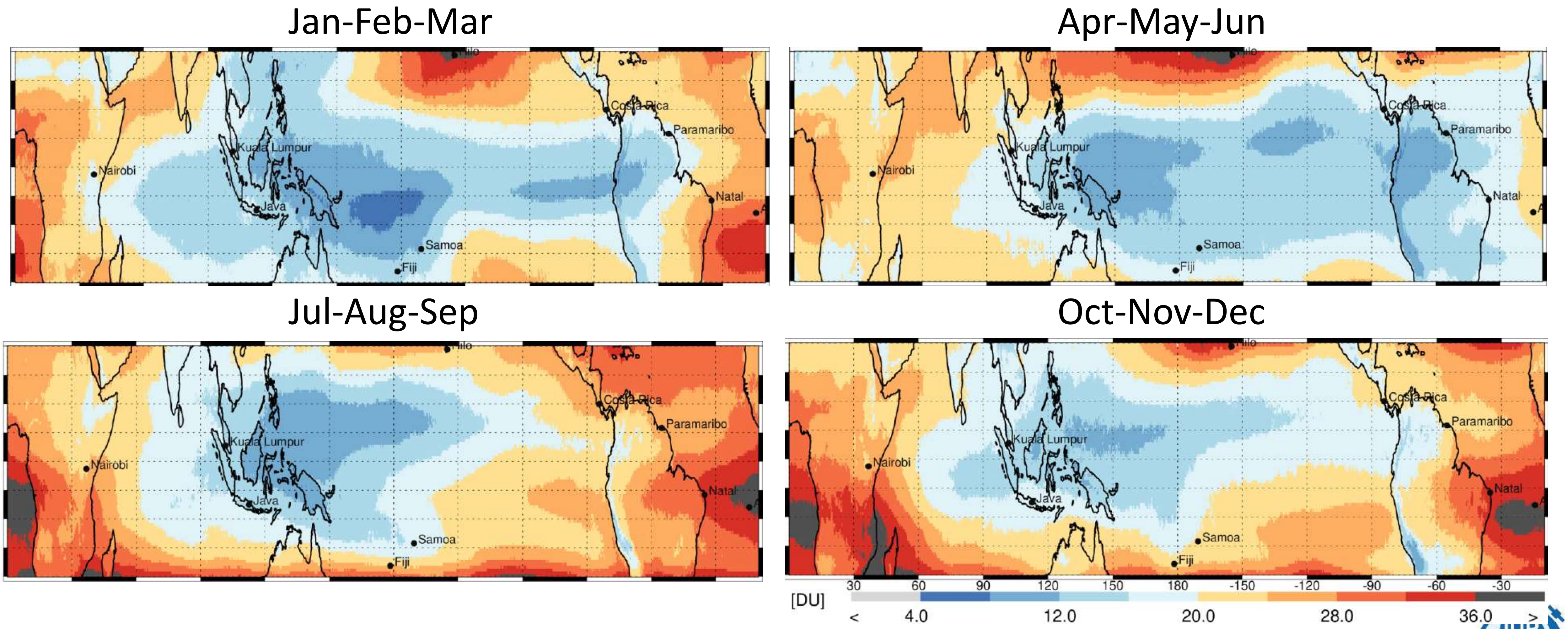

CHORA TTCO uncertainties

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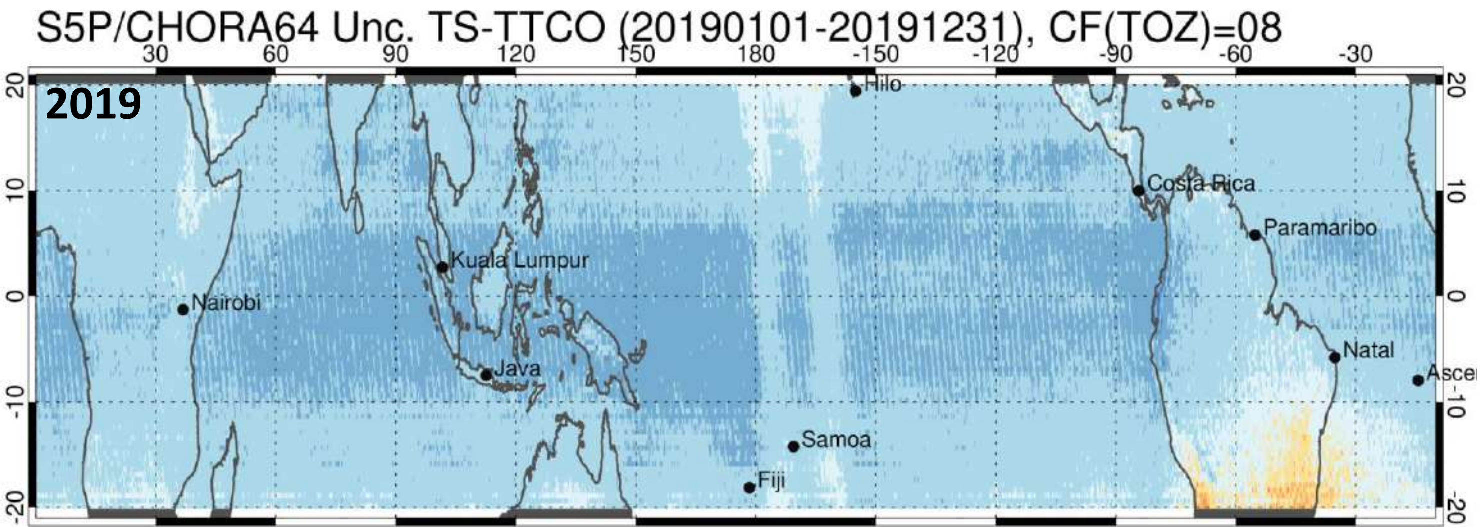
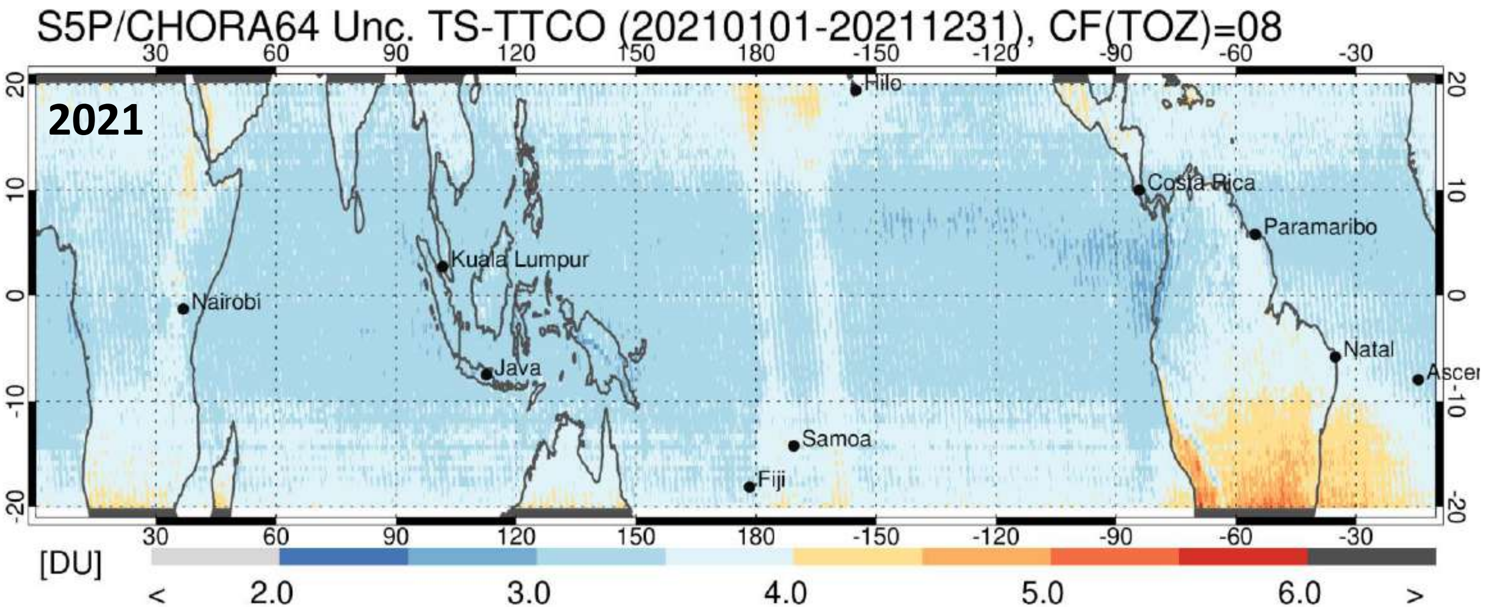
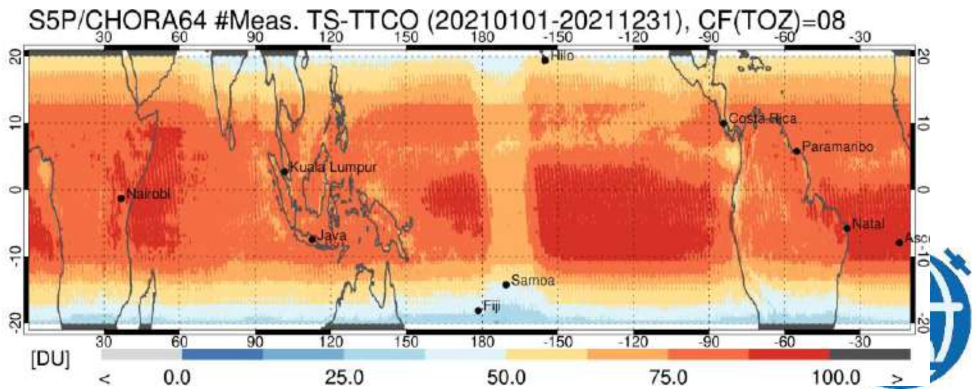


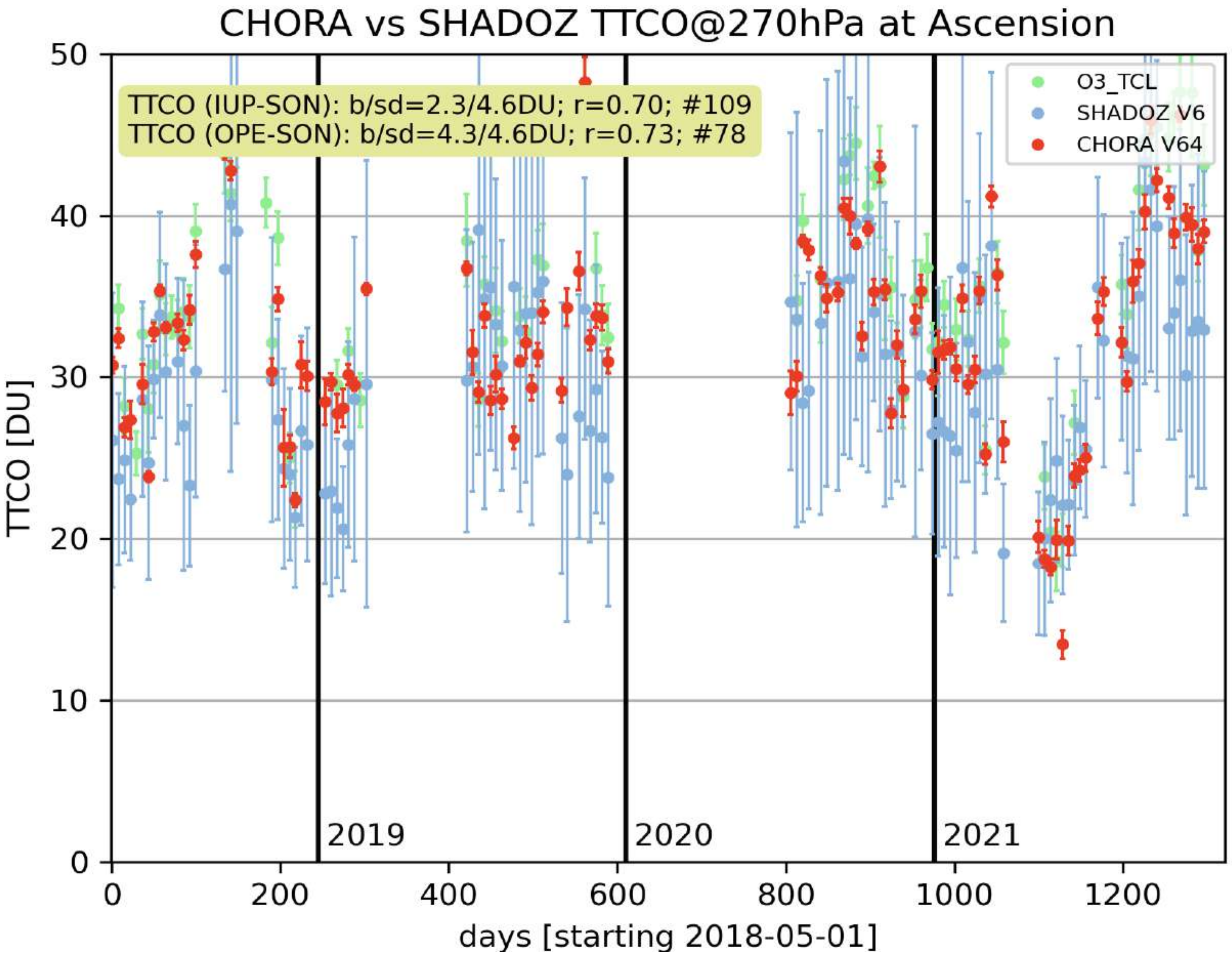


The TTCO uncertainty [DU] is calculated from spatial variations of TCO and ACCO.

- Uncertainty is lowest **[>2.5 DU]** in the inner tropics over the Pacific ocean and increases towards the extra-tropics. It is slightly higher over land, especially over South America **[>5 DU]**.
- The increase at the **date line** between 160°-180° is due to not collecting all orbits that cover the full globe. This is avoided in V7 by adding an extra orbit in the daily retrieval (#meas, fig below).
- The **uncertainty increases** from 2019 to 2021. Whether this is due to degradation of the instrument or to the version changes over mission lifetime needs to be further analysed.



CHORA validation with SHADOZ ozone sondes: e.g. Ascension



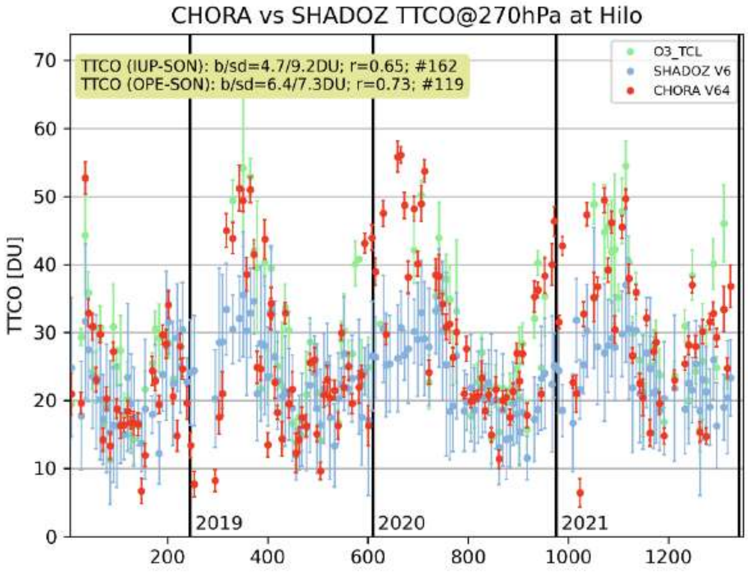
Ascension is located where the maximum ozone tropospheric columns are found.

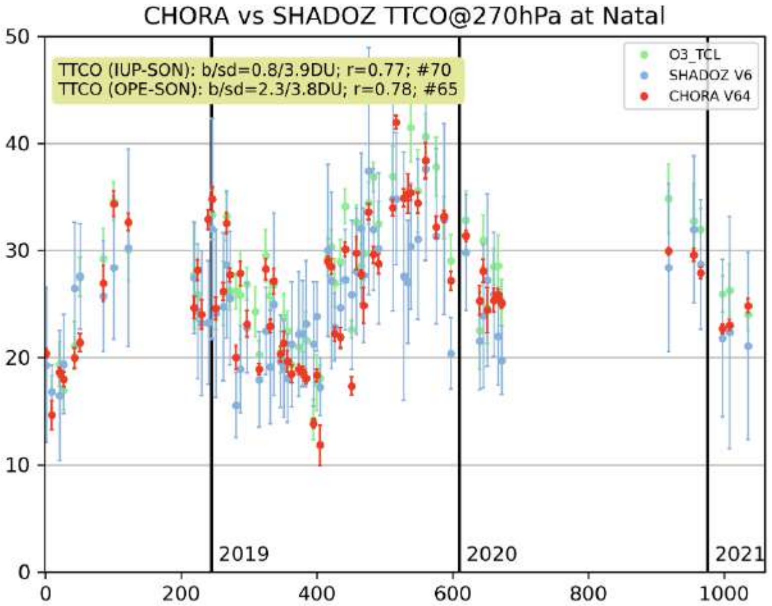
The natural variations are rather high as shown by the spread of SHADOZ data.

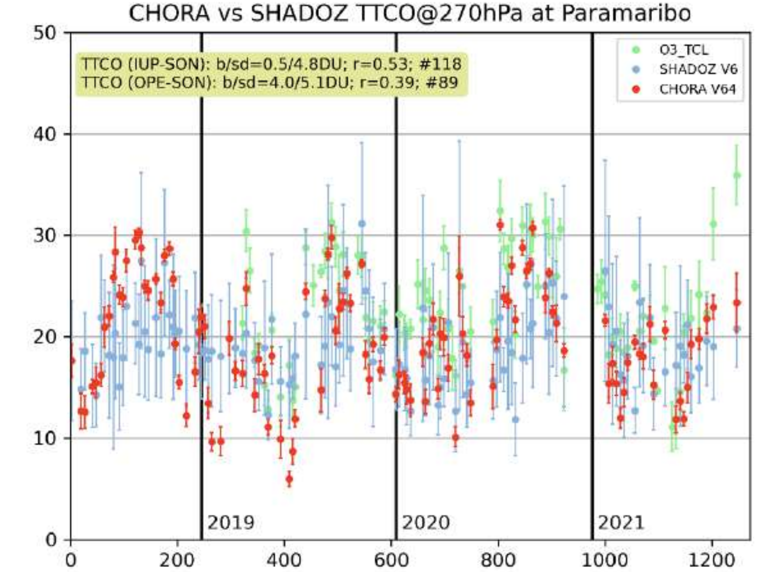
Both the operational (OPE) and CHORA (IUP) products have a similar spread of 4.6 DU and correlation of about 0.7 in comparison to ozone sondes.

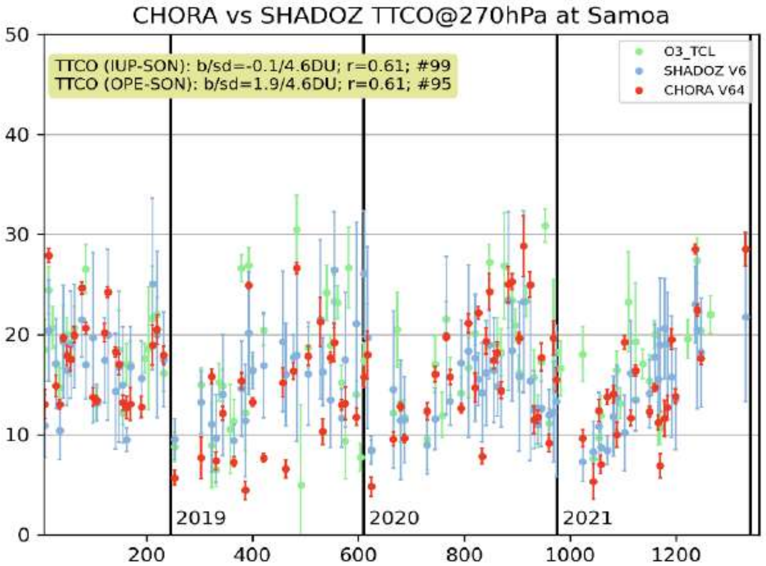
Due to the optimization steps the IUP product show a decrease in bias. But both products are within the mission requirements.

CHORA validation with SHADOZ ozone sondes: other stations









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CHORA 6.4/7.0 vs SHADOZ 6.0 ozone tropospheric columns

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CHORA V6.4 (PS)/7.0 (TR) TTCO@270hPa from O3L2 OFFL data and nearest collocation grid box. **Input: TOZ(CF<0.8), ACCO(CF>0.8).** ACCO grid step/size: **0.5°/1°. Output:** TOZ grid size: 0.5°x**0.25**°. Time range 2018/05 – 2022/06.

Data: S5P O3 OFFL/RPRO 01.01.07-02.03.00 (May 2018 – May 2022).
9 SHADOZ V6.0 sites: Ascension, Hilo, Costa Rica, Fiji, Kuala Lumpur, Nairobi, Natal, Paramaribo, Samoa.

CHORA – SONDE : TTCO relative difference [%]				
Version	Mean	SD(1σ)	Pearson	#Collocations
V6.4	4.2	21	0.67	672
Low/high [%]	0/7	24/16	-	310/362
V7.0	**6.9**	20	0.67	672
Low/high [%]	4/9	23/16	-	310/362

CHORA-PS 7.0 (TR) has a higher bias than **6.4 (CH)** which uses the CS/CHOVA monthly mean VMRs for the ozone/cloud height correction.

V7.0 is independent of external cloud correction data and thus also used in the next upgrade of **CHORA-LCT 7.0** that takes cloud information from nearest occurences.

Postprocessing of the ACCO height correction is used on both versions to increase number of retrievals and reduce scatter.

3. Outlook: CHO**R**A-LCT 7.0

Check the operational O3TCL product, part 2

Local cloud /TS-regression: See poster 51 by S. Satheesan

Comparisons with NASA/GSFC SHADOZ ozone sondes

CHORA (Cloud Height and Ozone Reference Algorithm): IUP processor / LCT=Local cloud Theil-sen-regression

CCDs vs ozone sonde data

Processors	7.0 CHORA-PS	O3TCL(OPE)	ROCVR #16
Bias [%]	6.9	15.7	17
Dispersion [%]	20	27.4	26
Pearson-R	0.67	0.58	
#Collocation	672	484	~800

VDAF operational data used for collo-cated comparison

Reported op. Data values (D. Hubbert)

Versions 7.0 are independent of climatologies for ozone height correction.

LCT: Potential to go to the extratropics, first comparisons show good results (see Poster 51).

(*) The 7.0 PS/LCT results are based on monthly mean comparisons which **reduces the natural variability** (dispersion) and **increases the correlation** (Pearson-R). Bias should not be affected.

Remarks: The differences of CHORA-PS+ and CHORA-PS* are due to the post-processing ACCO computation. CHORA-PS* is simply a comparison tool.

4. Conclusions:

The two IUP processors (CCD, CS) have improved over the last 5 years of mission.

While CS/CHOVA VMR monthly data is used in the previous CCD/CHORA version 6.4, it is directly implemented into CHORA 7.0. CHORA-PS 7.0 is an independent, stand-alone processor.

The need to **expand the latitudinal boundaries** into the extra-tropics (e.g. for GEO satellites like GEMS) lead to the ongoing development of CHORA-LCT (S.Satheesan) that uses cloud input data from neighbouring clouds to the retrieval pixel.

Comparisons with NASA/GSFC SHADOZ ozone sondes show low biases in all products (CHOVA <1%, CHORA-PS 7%, CHORA-LCT -6%).

The operational O3TCL product have similar correlation coefficients, slightly higher dispersion and in comparison to CHORA-PS a higher bias (7->16%).

CHORA (Cloud Height and Ozone Reference Algorithm): IUP processor / LCT=Local cloud Theil-sen-regression