

SSP MPC



Validation of S5P tropospheric ozone OFFL v01.01.02 using ozonesonde data

Daan Hubert¹, Arno Keppens¹ and Jean-Christopher Lambert¹

Acknowledgements to A. M. Thompson², J. C. Witte^{2,3}, B. J. Johnson⁴ and all SHADOZ contributing stations and instrument PI's Thanks to K.-P. Heue⁵, D. Loyola⁵ and K.-U. Eichmann⁶ for useful discussions



(1) Royal Belgian Institute for Space Aeronomy (BIRA-IASB), BE (2) NASA GSFC, USA (3) SSAI, USA (4) NOAA, USA (5) DLR, DE (6) IUP Bremen, DE

Co-funded by ESA S5P MPC and BELSPO/BIRA-IASB





28 Sep 2018

S5P Data Release Telecon

belspo







- L2_O3_TCL OFFL v01.01.02 from ESA HUB
 - Covers : 7 Nov 2017 12 Sep 2018
 - ignored v01.01.01 (Jul), mostly overlap with v01.01.02
 - Discard products that [do not span 5±0.5 day] OR [have double start and/or end date]
 → removes 59/298 products (=19.8%) of products.
- Follow PRD recommendation to remove all grid cells
 - CCD tropo column : qa_value<0.5
 - CSA upper tropo VMR : upper_tropo_flag>0

FRM data record : ozonesonde



In-situ reference data from SHADOZ & NOAA ozonesonde archives

- Vertically resolved O3 profiles from surface to ~30km
- 9 sites with \sim (bi)weekly sounding during S5p period, N=193 profiles.
- Data are very well characterized (Witte et al., 2017, 2018; Thompson et al., 2018; ...)
- Screening described in Hubert et al. (2016).
- Convert each sonde profile to S5p like information
 - CCD = partial O3 column between surface and 270 hPa,
 - CSA = mean O3 VMR over variable pressure range in upper troposphere.







CCD OFFL v01.01.02

Tropospheric ozone column (surface-270 hPa) 0.5° lat x 1° lon x 3 days





Issue #1: clear artificial latitudinal structure.



- Latitudinal structure seen in both tropospheric column and stratospheric reference column.
- These occur everywhere, but more often >15° latitude. They persist over several few days, but not longer.
- In all products, I noted band-to-band difference of 2 DU (= \sim 10%) and more.
- Is this caused by a latitudinal dependence in the Pacific reference region of (a) sampling uncertainty and/or (b) L2_O3 retrieval for very cloudy, opaque and high cloud pixels.

belspo Cesa

Issue #2 : spatial structure follows orbital sampling?



- Occasionally, there are striking matches between the spatial structure of CCD columns and the S5P swath.
- Is this an indication of sampling uncertainty of binned, cloud-free L2_O3 data?

belspo

eesa

Issue #2 : spatial structure follows orbital sampling?



- Occasionally, there are striking matches between the spatial structure of CCD columns and the S5P swath.
- Is this an indication of sampling uncertainty of binned, cloud-free L2_O3 data?

belspo

Cesa

Issue #3: incorrect CCD time windows



28 Sep 2018

- PRF recommends users to add +1 day to CCD time window (3 day) if stratospheric time window (~5 days) starts before midnight UTC.
- This is a good recommendation in most but not all cases \rightarrow needs further refinement.
- In a next release, this should be implemented at L2. It should not be the user's responsibility.





Issue #4: Unusual coverage





 About 5 products (March 2018) have a very unusual screening pattern.







- Time series of tropospheric ozone columns for **S5P OFFL v01.01.02** (3 day) and **ozonesonde** (single flight).
- All data are shown.

S5p CCD

Oct

(18.25S, 178.50E)

Aug

30

20

10

Suva

Dec/17

(18.13S, 178.40E, 6m

Feb/18

Apr

Jun

- Seasonal cycle is present, zonal wave-one pattern as well. •
- Signs of \sim 2-3 week cycles in S5P record are not verifiable using sonde.





• Most direct comparison.

S5p CCD (18.25S, 178.50E)

Aug

Oct

20

10

Suva

Dec/17

(18.13S, 178.40E, 6m)

Feb/18

Apr

Jun

• Caveat : (temporal) sampling of sonde is very low.





S5p CCD

Oct

(18.25S, 178.50E)

Aug

-40

-60

-80

Suva

Dec/17

(18.13S, 178.40E, 6m)

Feb/18

Apr

Jun

- S5p overestimates wrt sonde, by ~20% at many sites.
- Spread in comparisons between 12-43%.





S5p CCD

Oct

(18.25S, 178.50E)

Aug

-10

-15

-20

Suva

Dec/17

(18.13S, 178.40E, 6m)

Feb/18

Apr

Jun

- S5p overestimates wrt sonde, by ~3.6 DU.
- Spread in comparisons between 3-8 DU.

Conclusions CCD : OFFL v01.01.02



- Almost each product contains artificial (lat x lon) structures
 - How can this be mentioned in the PRF?
 - Refine sampling / gridding scheme?
- The recommendation to shift the time window works very well, but is not perfect. TODO : Fix this in a future release!
- Comparison of 239 S5p products to 193 ozonesonde profiles shows
 - Positive bias for S5p at all SHADOZ sites, about +20%.
 - Comparison spread of ~10-40%.
 - No change in quality during incorrect irradiance period (Apr-May).
 - (Caveat : sampling properties are very different.)



Conclusions CCD : OFFL v01.01.02



Assessment wrt product requirements

- Bias : close to required 25%. But not met at 3/9 sites!
- Random : required 10% clearly smaller than observed spread, but the difference in temporal sampling may contribute substantially.
- More consolidated assessment will be possible once SHADOZ archive has been updated (end 2018?).

Recommendation : release!

But with clear disclaimer (spatial artefacts, bias, spread) in PRF.





CSA OFFL v01.01.02

Upper tropospheric ozone mixing ratio (variable pressure range) 5° lat x 20° lon x 5 days







Spatial patterns in upper tropo VMR less well resolved than CCD tropospheric column

- VMR is consistently larger above Pacific than over Atlantic region, reflecting the wave-one pattern in tropical ozone.
- Some regions have very few measurements (e.g., S Atlantic, E Pacific).
- Difficult to see any clear deficiencies from these maps, the matched SAT-GND difference time series are crucial.



S5P Data



Oct

Feb/18

Apr

Jun

Aug

Dec/17







5 p CSA

Oct

(17.50S, 170.00E)

Aug

-60

-80

Suva

Dec/17

(18.135)178.40E, 6m)

Feb/18

Apr

Jun

Spread in comparisons between 20-59%.





S5p CSA

Oct

(17.50S, 170.00E)

Aug

Suva

(18.13)

Dec/17

S 178.40E, 6m)

Feb/18

Apr

Jun

-20

• Spread in comparisons between 9-19 DU.





- Comparison of 239 S5p products to 193 ozonesonde profiles shows
 - Negative bias for S5p at all SHADOZ sites, about -30%.
 - Comparison spread of ~20-60%.
 - No change in quality during incorrect irradiance period (Apr-May).
 - (Caveat : sampling properties are very different.)



Conclusions CSA : OFFL v01.01.02



Assessment wrt product requirements No requirements for VMR expressed, use those for column instead.

- Bias : worse than required 25%, at 5/6 sites.
- Random : required 10% clearly smaller than observed spread, but the difference in temporal sampling may contribute substantially.
- More consolidated assessment will be possible once SHADOZ archive has been updated (end 2018?).

Recommendation : release?

Needs a very clear disclaimer (large bias & spread).

Assessment of user-friendliness of products

SSP MPC

Evaluation of how self-explanatory the .nc data files are for each tropospheric O3 product.

	Easy	Moderate	Hard
Latitude, longitude	CCD, CSA		
Time window	CSA	CCD	
Vertical range		CCD	CSA
O3 column / VMR	CCD, CSA		
O3 column / VMR uncertainty	CCD, CSA		
O3 data screening	CCD	CSA	
Influence quantities	CCD, CSA		

- Do variables and attribute names make sense?
- Does the file structure make sense?
- Should the user consult (a lot of) additional documentation to read out data correctly?
- Should s/he make (many) manipulations to correct for known issues?







Backup

S5P Data Release Telecon







S5P Data

Two S5p tropospheric ozone products, two types of information







CCD = convective cloud differential

O3 partial column from surface to 270 hPa, gridded 0.5° x 1° x ~3 days, cloud free cells

CSA = cloud slicing algorithm

mean O3 VMR in upper tropo (~190-425/550 hPa), gridded 10° x 20° x ~5 days, (very) cloudy cells





- In-situ measurement of O3 by ozonesondes at stations in SHADOZ network
- From surface to ~30km, at ~200m resolution
- Flights every ~1-2 weeks

Nov/17

Hilo (19.7°N, 155.1°W, 11m)

Nairobi (1.3°S, 36.8°E, 1795m) Natal (5.8°S, 35.2°W, 32m)

Samoa (14.2°S, 170.6°W, 82m) Suva (18.1°S, 178.4°E, 6m)

Heredia (10.0°N, 84.1°W, 1176m) Paramaribo (5.8°N, 55.2°W, 7m)

Sepang Airport (2.7°N, 101.7°E, 17m)

Ascension Island (8.0°S, 14.4°W, 79m)

• S5p matches : 8 (now), 144 (near future)

Dec

Jan/18



Jul

Jun

S5P Data Release Telecon

Apr

May

Mar

Feb

Oct

Sep

Aug

First remarks on ATBD v1.5 (draft)

- Ensure final parameter settings are correct
 - CSA fit range pressure
 - Screening
 - Averaging time windows
 - ...
- Clarify range of products
 - vertical : 200 or 270 hPa (CCD), 190-425/550 hPa (CSA)
 - temporal : 3/5 days tropo? uniform in window or asymmetric?
 - horizontal : ok

	Deutsches Zentrum für Luft- und Raumfahrt e.V. in der Helmholtz-Gemeinschaft	
TROPC ozone	OMI/S5P ATBD of tropos data products	pheric inel-5p



