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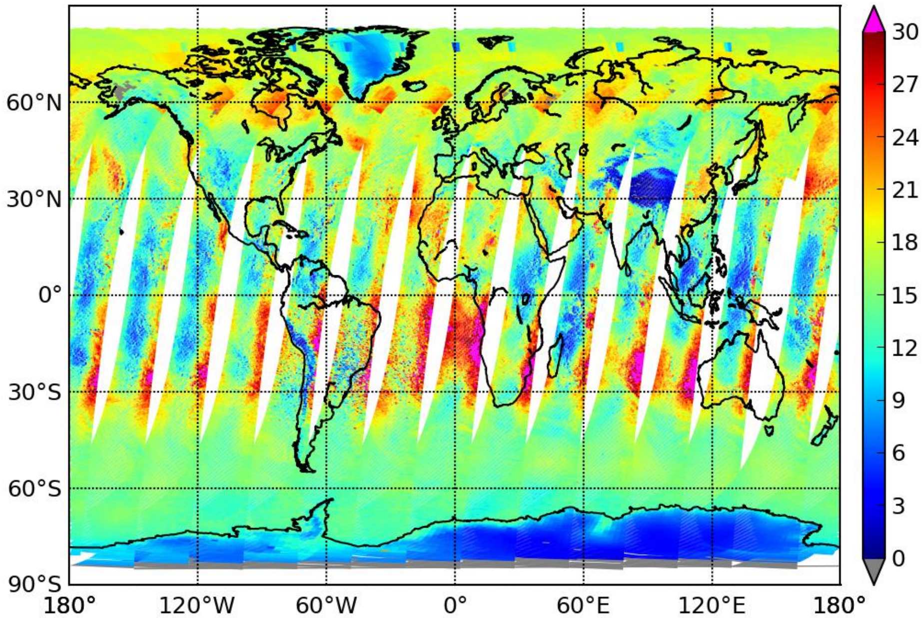
SAF/AC VALIDATION REPORT

Validated products:

Identifier	Name	Acronym
O3M-304	NRT Tropospheric Ozone, Ozone profiles, METOP-C	TrO/NHP
O3M-305	Offline Tropospheric Ozone, Ozone profiles, METOP-C	TrO/OHP



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Reporting period:	February 2019 – December 2019
Validation methods:	Balloon soundings
Input data versions:	Base Algorithm Version: 6.3
Data processor	Product Algorithm Version: 2.03
Versions:	Product Software Version: 2.02

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Acronyms and abbreviations

ATBD	Algorithm Theoretical Basis Document
GOME	Global Ozone Monitoring Experiment
MetOp	Meteorological Operational satellite
NDACC	Network for the Detection of Atmospheric Composition Change
NH	Northern Hemisphere
OPERA	Ozone Profile Retrieval Algorithm
PUM	Product User Manual
SH	Southern Hemisphere
SZA	Solar Zenith Angle
TrOC	Tropospheric integrated Ozone Column
WOUDC	World Ozone and UV Data Center

Introduction to EUMETSAT Satellite Application Facility on Atmospheric Composition monitoring (AC SAF)

Background

The monitoring of atmospheric chemistry is essential due to several human-caused changes in the atmosphere, like global warming, loss of stratospheric ozone, increasing UV radiation, and pollution. Furthermore, the monitoring is used to react to the threats caused by the natural hazards as well as follow the effects of the international proTrOCols.

Therefore, monitoring the chemical composition and radiation of the atmosphere is a very important duty for EUMETSAT and the target is to provide information for policy makers, scientists and general public.

Objectives

The main objectives of the AC SAF is to process, archive, validate and disseminate atmospheric composition products (O_3, NO_2, SO_2, BrO, HCHO, H_2O, OClO, CO, NH3), aerosol products and surface ultraviolet radiation products utilising the satellites of EUMETSAT. The majority of the AC SAF products are based on data from the GOME-2 and IASI instruments onboard Metop satellites.

Another important task besides the near real-time (NRT) and offline data dissemination is the provision of long-term, high-quality atmospheric composition products resulting from reprocessing activities.

Product categories, timeliness and dissemination

NRT products are available in less than three hours after measurement. These products are disseminated via EUMETCast, WMO GTS or internet.

- Near real-time trace gas columns (total and tropospheric O_3 and NO_2, total SO_2, total HCHO, CO) and high-resolution ozone profiles
- Near real-time absorbing aerosol indexes from main science channels and polarization measurement detectors
- Near real-time UV indexes, clear-sky and cloud-corrected

Offline products are available within two weeks after measurement and disseminated via dedicated web services at EUMETSAT and AC SAF.

- Offline trace gas columns (total and tropospheric O_3 and NO_2, total SO_2, total BrO, total HCHO, total H_2O) and high-resolution ozone profiles
- Offline absorbing aerosol indexes from main science channels and polarization measurement detectors
- Offline surface UV, daily doses and daily maximum values with several weighting functions

Data records are available after reprocessing activities from the EUMETSAT Data Centre and/or the AC SAF archives.

- Data records generated in reprocessing
- Lambertian-equivalent reflectivity
- Total OClO

Users can access the AC SAF offline products and data records (free of charge) by registering at the AC SAF web site.

More information about the AC SAF project, products and services: https://acsaf.org/
AC SAF Helpdesk: helpdesk@acsaf.org
Twitter: https://twitter.com/Atmospheric_SAF

1. Applicable SAF/AC Documents

[ATBD] Algorithm Theoretical Basis Document for Near Real Time and Offline Ozone profiles, KNMI/GOME/ATBD/01/001, issue 2.0.1, Olaf Tuinder, 20181115.

[PUM] Product User Manual for Near Real Time and Offline Ozone profiles, KNMI/GOME/PUM/001, issue 2.00, Olaf Tuinder, 20181115.

Both documents are available at http://acsaf.fmi.org in the *Documents* section.

2. General Introduction

This report contains validation results of the GOME-2C tropospheric ozone column product, retrieved by the Ozone Profile Retrieval Algorithm (OPERA) at KNMI. It covers the time period February 2019 until December 2019 for GOME-2C.

When comparing with the outcome of previous validation results (Delcloo, 2015), a degradation correction has been applied to all sensors (on MetOp-A, MetOp-B and MetOp-C) and an intercomparison with the results, reported in the operational report will be discussed (Operations Report, Issue 1/2020 rev. 1, 2020). Since these TrOC products are derived from the OPERA ozone profile product, it is possible to take into account the averaging kernels in the analysis. The outcome is summarized at the end of this report and contains an advice if these products meet the user requirements.

3. Validation of tropospheric ozone columns using ozonesondes

3.1 Introduction

The AC SAF GOME-2 tropospheric ozone column product validation was carried out using ozone profile measurements with balloon sounding data. Ozonesondes are lightweight balloon-borne instruments which are able to make ozone measurements from the surface up to about 30 km, with much better vertical resolution than satellite data. In general, also the precision and accuracy will be better, at least in the lower stratosphere and the troposphere. Another advantage is that ozone soundings can be performed at any time and at any meteorological condition.

The precision of ozonesondes varies with altitude and depends on the type of ozonesonde used. Table 1 below shows indicative precision (in percent) of the Electrochemical Concentration Cell (ECC), Brewer-Mast (B-M) and the Japanese KC79 ozonesondes, at different pressure levels of the sounding (taken from the AC SAF Science Plan).

Table 1: Precision of different types of ozonesondes at different pressure levels (%).

Pressure level (hPa)	ECC	B-M	KC79
10	2	10	4
40	2	4	3
100	4	6	10
400	6	16	6
900	7	14	12

It is shown from Table 1 that the profiles from ozonesondes are most reliable around the 40 hPa level, which is around the ozone maximum. The error bar of profiles from ozonesondes increases rapidly at levels above the 10 hPa level, which is around 31 km altitude. For this validation report, only the station of Hohenpeissenberg is using B-M sondes, all the other stations under consideration (Table 2) use ECC sondes, while KC-79 sondes are not launched anymore.

3.2 Dataset description

GOME-2 ozone data used in this validation report is from the beginning of February 2019 up to the end of December 2019. The level 1b algorithm version used for the GOME-2C tropospheric ozone products is 6.3**.**

GOME-2 tropospheric ozone column data was made available by KNMI at pre-selected sites. These sites correspond to sites where ozone soundings are performed on a regular basis. Data was made available by the World Ozone and Ultraviolet Data Center (WOUDC - http://www.woudc.org) and NILU's Atmospheric Database for Interactive Retrieval at Norsk Institutt for Luftforskning (NADIR - http://www.nilu.no/nadir/). However, since this report takes into account recently retrieved TROC data, it is not always possible for all the stations to have as much as ozonesonde data available to validate.

The statistics are shown in function of latitude belts. These are the belts taken into account:

Latitude belts from north to south:

1. Polar stations north: green (67N – 90 N)
2. Midlatitude stations north: black (30 N – 67 N)
3. Tropical stations: Red (30 N – 30 S)
4. Midlatitude stations south: grey (30 S – 70 S)
5. Polar stations south: blue (70 S – 90 S)

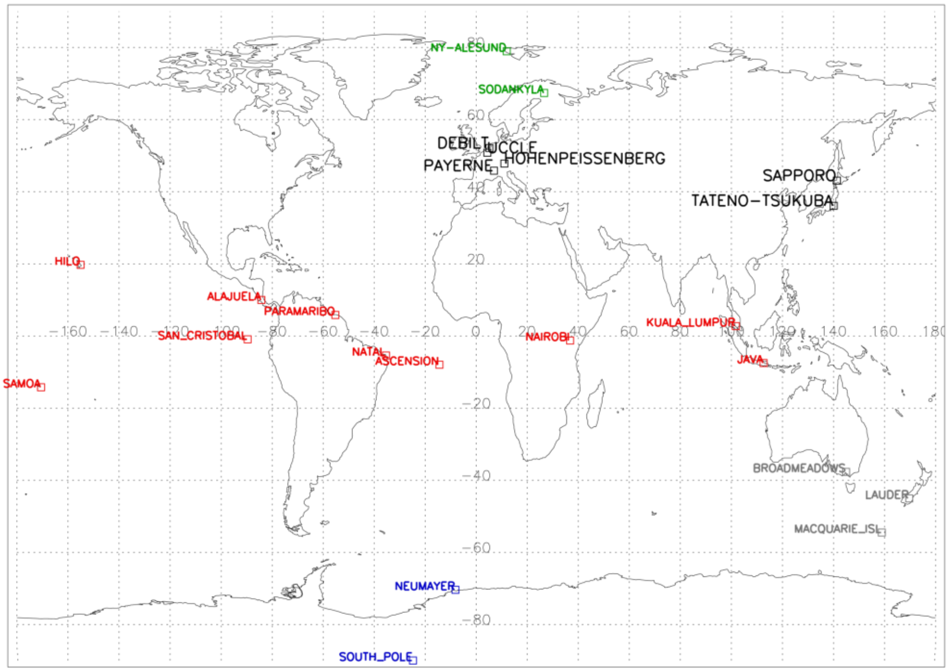


Figure 1: Stations used in the validation report.

Ozonesonde data are generally made available by the organization carrying out observations after a delay in order to leave time for necessary verification and correction of the data quality. Nevertheless, some organizations make their ozone profile data readily available for validation purposes. Figure 1 shows the stations used in this validation report.

The validation is performed in function of latitude belts. The number of ozonesondes, used for each station, is summarized in Table 2. The GOME-2 tropospheric ozone column data taken into consideration are the ones which have received the quality processing status of “Overall convergence, successful retrieval”. More details about the quality flags can be found in the PUM document (Product User Manual for the Near Real Time and Offline Ozone Profile), pages 22-23.

Table 2: Overview of the stations taken into account with the numbers of ozonesondes used in the analysis and the last day, an ozonesonde was available for the intercomparison.

STATION	Longitude	Latitude	Nr of sondes	Last day available ozonesonde
ASCENSION	-7.98	-14.42	7	20-Feb-19
BROADMEADOWS	-37.69	144.95	50	18-Dec-19
DEBILT	52.1	5.18	50	27-Dec-19
FIJI	-18.1	178.4	1	25-Jan-19
HILO	19.717	-155.083	9	28-Feb-19
HOHENPEISSENBERG	47.8	11.02	128	30-Dec-19
IRENE	-25.9	28.22	4	6-Mar-19
LAUDER	-45.045	169.684	31	25-Jul-19
LERWICK	60.14	-1.19	25	3-Jul-19
MACQUARIE_ISL	-54.5	158.94	47	31-Dec-19
NAIROBI	-1.27	36.8	9	28-Feb-19
NEUMEYER	-70.39	-8.15	55	24-Dec-19
NY-ALESUND	78.93	11.95	73	30-Dec-19
PARAMARIBO	5.81	-55.21	16	25-Jun-19
PAYERNE	46.817	6.95	33	29-Mar-19
SAMOA	-14.23	-170.56	2	28-Feb-19
SODANKYLA	67.3666	26.6297	19	17-Jun-19
SOUTH_POLE	-89.99	-24.8	19	30-Jul-19
TATENO-TSUKUBA	36.1	140.1	39	29-Nov-19

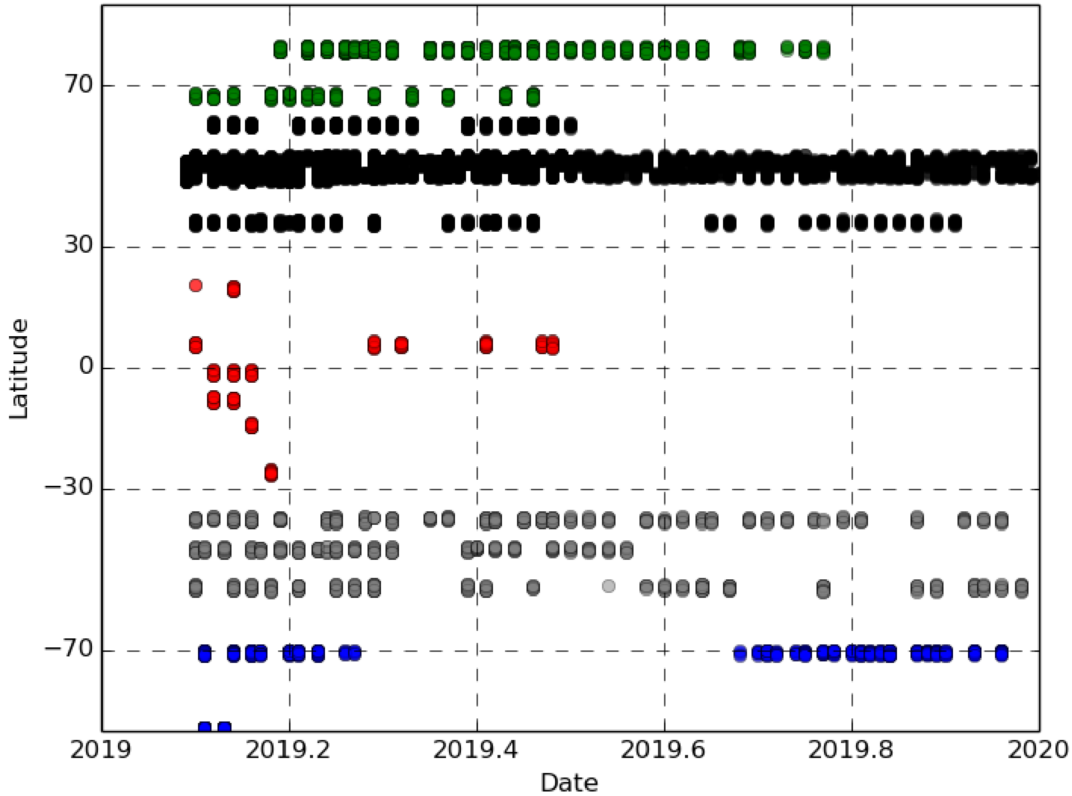


Figure 2: Spatial and temporal representation of the collocation data used for the validation with ozonesonde data for the time period February 2019 – December 2019 (Latitude-time sampling of co-locations).

3.3 Co-location criteria

The selection criteria, taken into account are twofold:

- The geographic distance between the GOME-2 pixel center and the sounding station location is 100 km.
- The time difference between the pixel sensing time and the sounding launch time is the second criterion and is fixed at ten hours of time difference. Each sounding that is correlated with a GOME-2 overpass is generally correlated with several GOME-2 pixels if the orbit falls within the 100 km circle around the sounding station. This means that a single ozone profile is compared to more than one GOME-2 measurement.

The spatial and temporal representation of the collocation data, used for the validation is shown in Figure 2: Spatial and temporal representation of the collocation data used for the validation with ozonesonde data for the time period February 2019 – December 2019 (Latitude-time sampling of co-locations).

3.4 Ozone sounding pre-processing

GOME-2 ozone profiles are given as partial ozone columns on 40 varying pressure levels, calculated by the Ozone Profile Retrieval Algorithm (OPERA) developed by KNMI. Ozone partial columns are expressed in Dobson Units.

Ozonesondes measure the ozone concentration along the ascent with a much higher vertical resolution than GOME-2. Ozonesondes have a typical vertical resolution of 100m while GOME-2 profiles consist of 40 layers between the ground and 0.001hPa. Ozonesondes give the ozone concentration in partial pressure. The integration requires some interpolation, as GOME-2 levels never match exactly ozonesonde layers. (Delcloo and Kins, (2009, 2012))

For the comparison, ozonesonde profiles are integrated between the GOME-2 pressure levels of the GOME-2 profile being compared. This means when a single ozonesonde profile is compared to different GOME-2 profiles, the actual reference ozone values are not the same given that the GOME-2 level boundaries vary from one measurement to another. The derived tropospheric ozone column product ($X_{GOME\text{-}2}$) is the sum of the layers until the defined level. More information on how this level is defined for both TrOC products, is discussed in the next section.

In this report we also take into account the averaging kernels (AVK) of the GOME-2 ozone profile (Delcloo and Kins, (2009, 2012); Rodgers, 1990). The motivation to apply the AVK is to "smooth" the ozone soundings towards the resolution of the satellite, to look at the GOME-2 profiles with "the eyes" from the satellite. Equation (1) shows how the kernels have been applied.

$$X_{avk\_sonde} = X_{apriori} + A\,(X_{raw\ sonde} - X_{apriori}) \qquad (1)$$

Where A represents the averaging kernel, X_{avk_sonde} is the retrieved ozonesonde profile, X_{raw_sonde} is the ozonesonde profile and $X_{apriori}$ is the a-priori profile.

4. Results

This report will communicate the results for two methods in order to retrieve the tropospheric ozone columns (TrOC).

The first method derives the TrOC by deriving the tropopause height from the ECMWF temperature profile. This method aims to extract the 'true' tropospheric ozone column; the atmosphere is separated vertically into two regimes by the presence of a temperature inversion that prevents the mixing of air between troposphere and stratosphere. This inversion layer is called the tropopause. The height of the tropopause varies, depending on the latitude, season and regional effects of large scale meteorological systems. The tropopause height definition used by the World Meteorological Organization is: "The lowest level at which the lapse rate decreases to 2 °C/km or less, provided that the average lapse rate between this level and all higher levels within 2 km does not exceed 2 °C/km" [WMO Manual on Codes, Vol. I. 1-A, WMO–No. 306]. When the tropopause level is defined, the TrOC is then defined as the sum from the layers below the defined level. More information can be found in the ATBD. Although this extraction method for TrOC is straightforward, it also introduces easily errors, related to stratosphere-troposphere exchange processes.

Therefore, a second derived product is proposed which takes into account the integrated tropospheric ozone until an altitude of about 500 hPa in order to avoid influences of stratospheric ozone in the TrOC product. This product could also be useful as a boundary condition product for chemical transport models (CTM) in an operational context, since it only takes into account the lower troposphere (until 500 hPa).

To calculate the relative differences of the tropospheric ozone column product, we apply:

$$(X_{GOME\text{-}2} - X_{AVK\text{-}SONDE})/X_{AVK\text{-}SONDE} \quad (2)$$

Where $X_{GOME\text{-}2}$ represents the integrated tropospheric ozone until the level below the tropopause height and $X_{AVK\text{-}SONDE}$ is the associated integrated smoothed ozonesonde profile.

The tropospheric ozone column (TrOC) product has the following user requirements:

- Threshold accuracy: within 50 %,
- Target accuracy: within 20 %
- Optimal accuracy: within 15 %

In the next two subsections the results for both methods will be reported.

4.1 Statistics for the tropopause product

Table 3 describes some general statistics for the GOME-2C dataset.

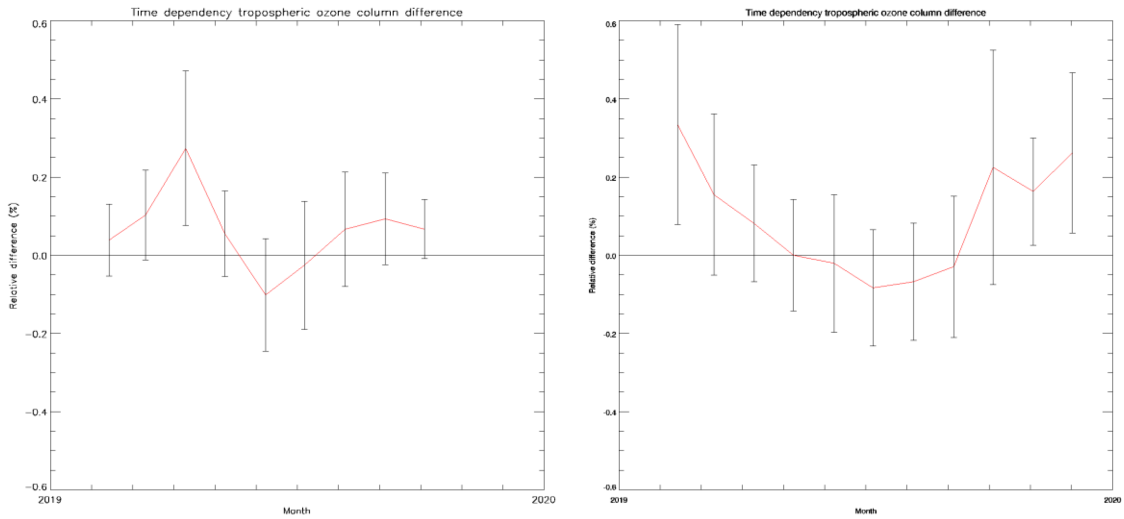
Table 3: Relative Differences (RD) and standard deviation (STDEV) are shown (in percent) on the accuracy of the GOME-2 tropospheric ozone column products for different latitude belts, validated against X ***$X_{AVK\text{-}sonde}$.***

	GOME-2C			
February 2019 – December 2019	**RD (%)**	**STDEV (%)**	**AD (DU)**	**STDEV (DU)**
northern polar regions	6.31	19.1	1.44	5.4
northern midlatitudes	10.6	23.91	2.48	6.7
tropical regions	27.99	27.46	6.5	6.36
southern midlatitudes	15.25	21.07	2.98	4.6
southern polar regions	11.27	54.82	0.93	4.36

The statistics reveal that the GOME-2C Tropospheric Ozone Column product is after comparison with balloon sounding ozonesonde data within the target accuracy (20 %), except for the tropical region. Please notify, that for the tropical stations only 6 months of data are available.

4.1.1 Seasonal dependency

Figure 3 shows the relative differences (%) on a monthly basis between the GOME-2C tropospheric ozone columns compared with the ozonesondes for 4 different latitude belts for the time period February 2019 – December 2019. There is a clear seasonal cycle present in the dataset.



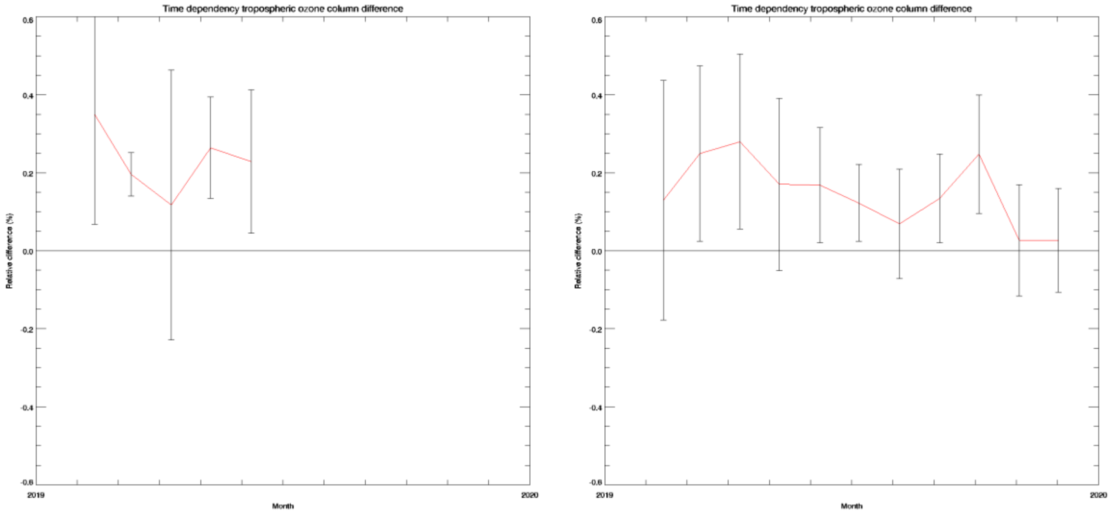
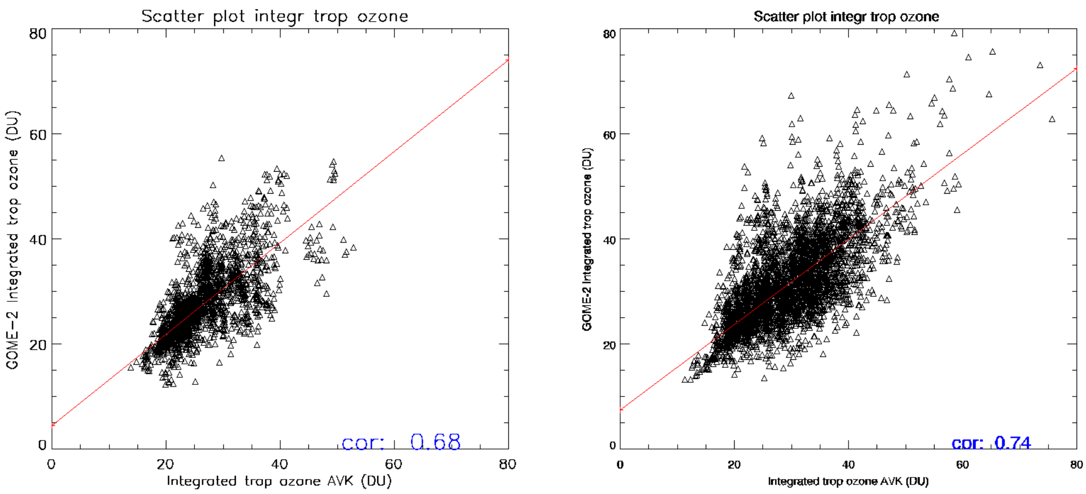


Figure 3: Relative differences (%) between GOME-2C tropospheric ozone column (tropopause related) compared with the ozonesondes for 4 different latitude belts (N-polar (ul), N-midlatitudes (ur), tropical (ll) and S-midlatitudes (lr)) for the time period February 2019 – December 2019.

4.1.2 Scatter plots

To verify the skill of the tropospheric ozone column product more thoroughly, some scatter plots of the different versions are shown in Figure 4. They illustrate the integrated tropospheric GOME-2C ozone concentrations against the smoothed ozonesonde data for the fixed altitude products. Also the correlation is shown, which varies between 0.68 for polar stations till 0.86 for midlatitude stations.



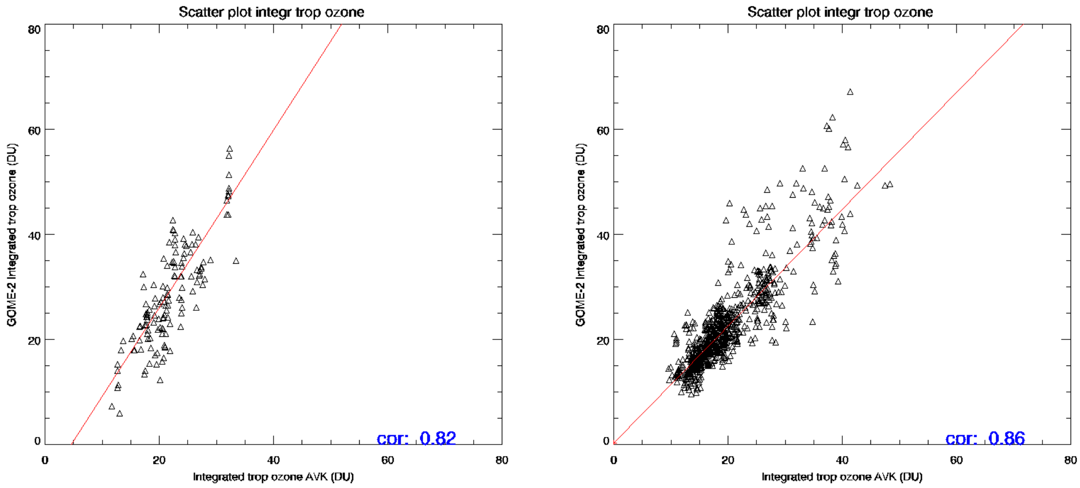


Figure 4: Scatter plots for the GOME-2C tropospheric ozone column products for 4 different latitude belts (N-polar (ul), N-midlatitudes (ur), tropical (ll) and S-midlatitudes (lr)) for the time period February 2019 – December 2019 (tropopause product), applying the kernels.

4.1.3 Scan angle dependency

When looking at the operational plots, it is obvious that there must be a scan angle dependency. (e.g. for GOME-2C: Figure 9 and Figure 10). This has been verified by taking a closer look at this dependency. Figure 5 reveals that there is a clear east-center-west dependency. The center pixel shows the lowest bias for all latitude belts, except for the southern polar stations. The east and west scan show more elevated ozone concentrations, except for the southern polar stations.

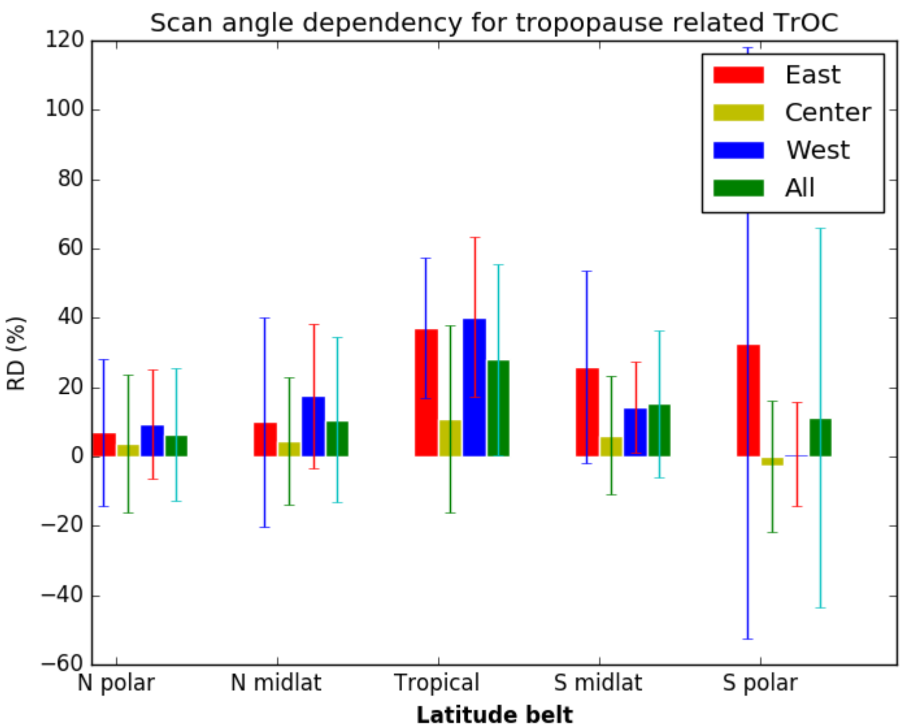


Figure 5: Scan angle dependency for tropopause related TrOC product

4.2 Statistics for the fixed altitude product

Compared to the tropopause related product, the retrieved TrOC ozone is the integrated ozone profile **until** an altitude of **500 hPa**.

Table 4 describes some general statistics for the GOME-2Cdatasets.

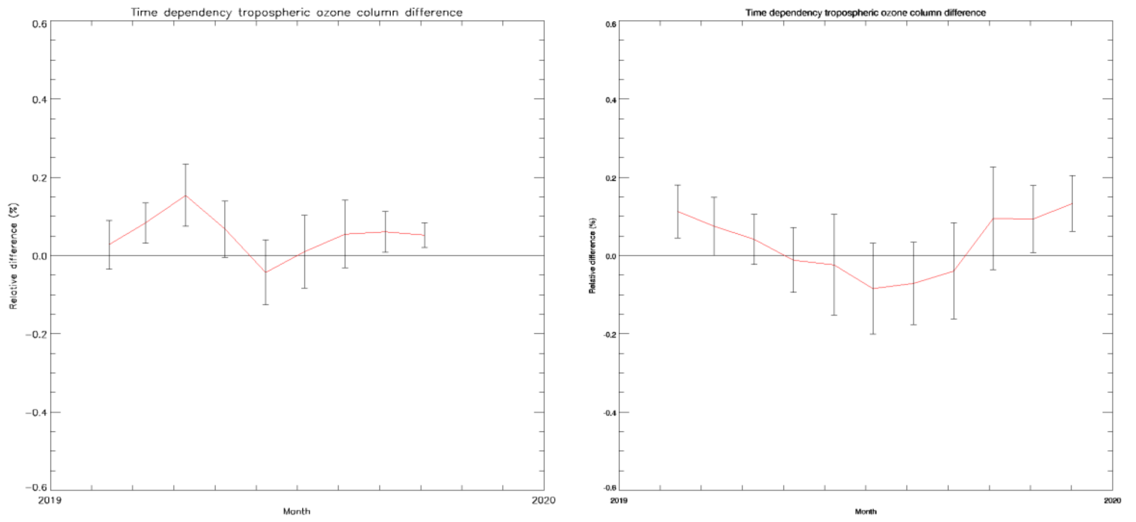
Table 4: Relative Differences (RD) and standard deviation (STDEV) are shown (in percent) on the accuracy of the GOME-2 tropospheric ozone column products for different latitude belts and for different products, validated against $X_{AVK\text{-}sonde}$.

	GOME-2C			
February 2019 – December 2019	**RD (%)**	**STDEV (%)**	**AD (DU)**	**STDEV (DU)**
northern polar region	5.43	10.06	0.9	1.7
northern midlatitudes	3.27	12.1	0.4	2.14
tropical region	15.06	28.63	1.44	2.63
southern midlatitudes regions	8.83	13.76	1.02	1.55
southern polar region	-2.77	10.89	-0.27	1.04

It is shown that all fixed TrOC products are within the target value (20 %). Please notify, that for the tropical stations only 6 months of data are available.

4.2.1 Seasonal dependency

Figure 6 shows the relative differences (%) on a monthly basis between the GOME-2C tropospheric ozone columns compared with the ozonesondes for 4 different latitude belts for the time period February 2019 – December 2019. Also here the seasonal behavior is present in the data.



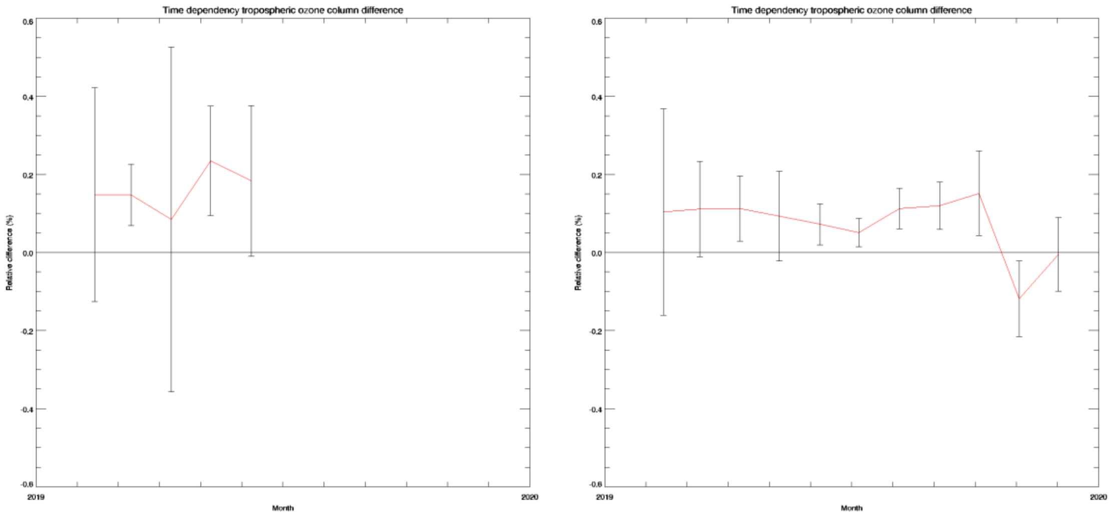
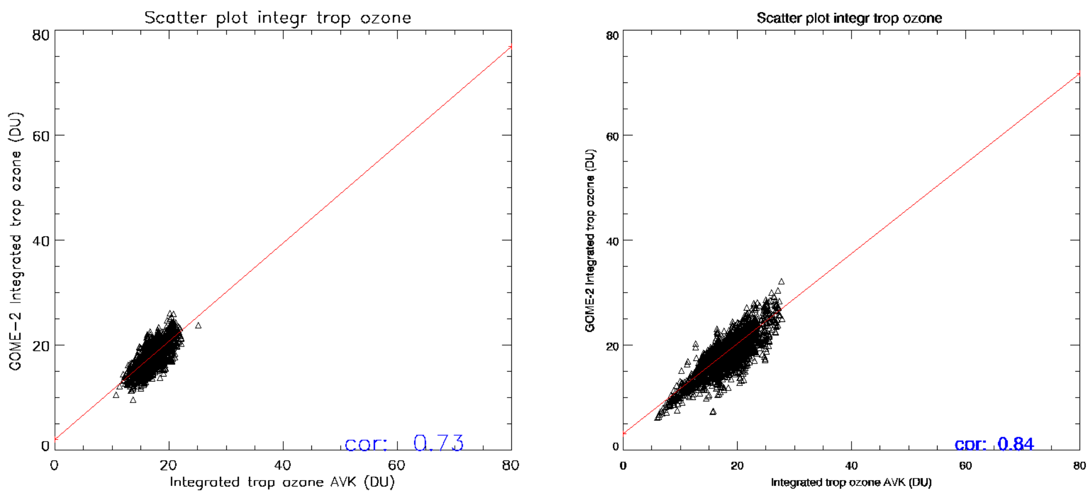


Figure 6: Relative differences (%) between GOME-2C tropospheric ozone column (fixed) compared with the ozonesondes for4 different latitude belts (N-polar (ul), N-midlatitudes (ur), tropical (ll) and S-midlatitudes (lr)) for the time period January 2019 – December 2019

4.2.2 Scatter plots

To verify the skill of the tropospheric ozone column product more thoroughly, some scatter plots of the different versions are shown in Figure 7. They illustrate the integrated tropospheric GOME-2 ozone concentrations against the smoothed ozonesonde data for the fixed altitude products. The same range in x and y axis has been chosen, to illustrate the difference in retrieved ozone concentrations between the tropopause related TrOC product (Figure 4) and the fixed TrOC product (Figure 7).



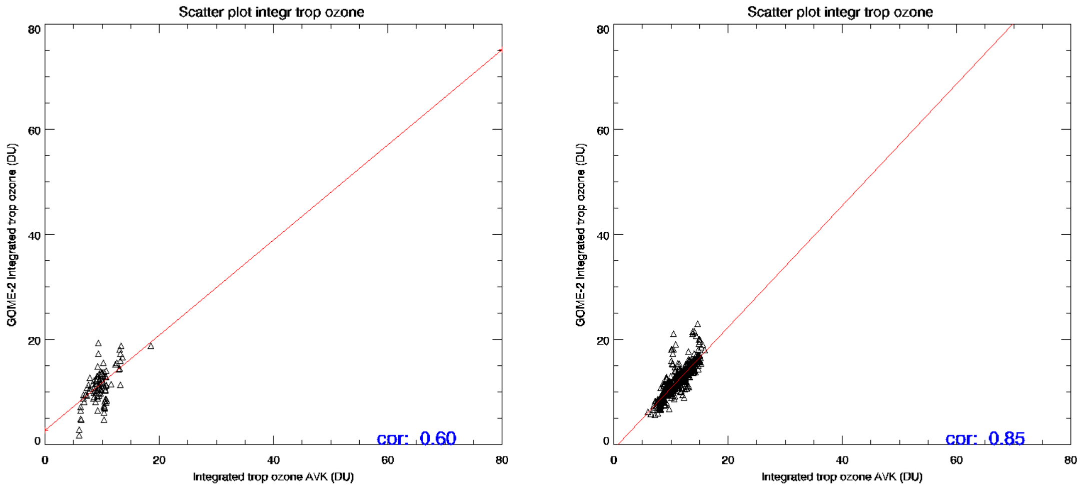


Figure 7: Scatter plots for the GOME-2C tropospheric ozone column products for 4 different latitude belts (N-polar (ul), N-midlatitudes (ur), tropical (ll) and S-midlatitudes (lr)) for the time period February 2019 – December 2019 (fixed product), applying the kernels.

4.2.3 Scan angle dependency

The operational plots reveal a scan angle dependency. (e.g. for GOME-2C: Figure 9 and Figure 10). Also here the dependency on scan angle has been verified in Figure 8, which reveals that also here the center pixel shows in general the lowest bias, except for the southern polar stations.

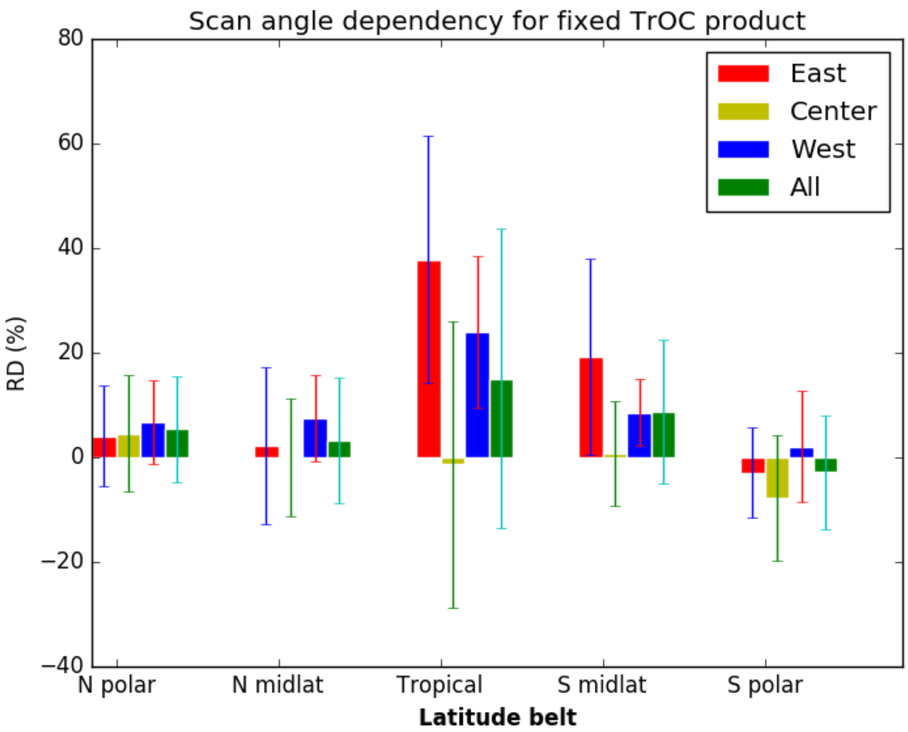


Figure 8: Scan angle dependency for fixed related TrOC product.

5. Examples of global output

To show that the tropospheric ozone column product has skill to identify elevated tropospheric ozone concentrations within the defined tropospheric ozone layers (tropopause related TrOC product and fixed altitude TrOC product) some examples are shown in the Figure 9 and Figure 10 for the 28th of September 2019 from GOME-2C.

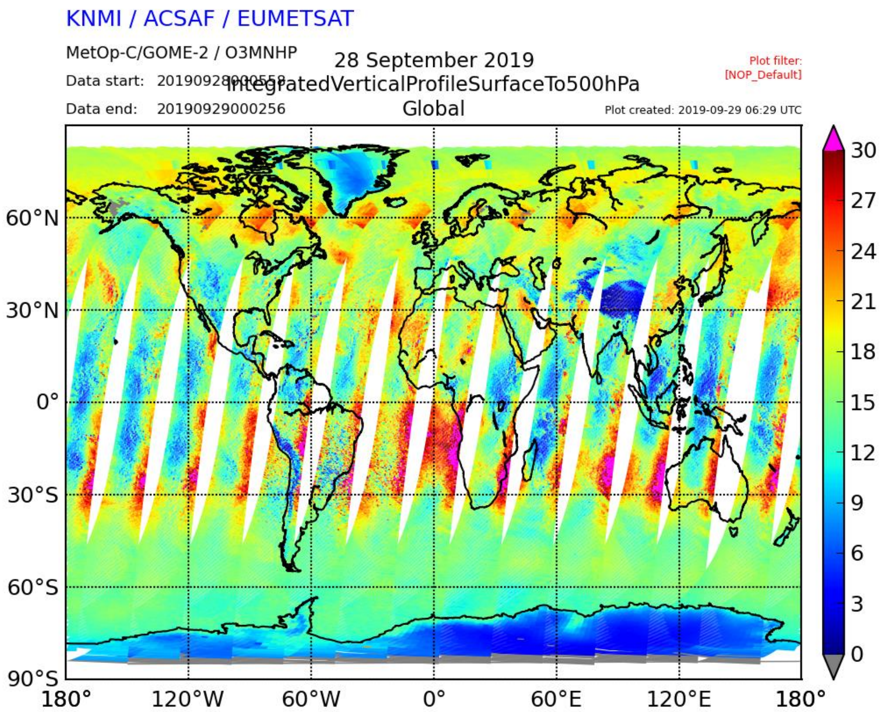


Figure 9: Vertical integrated ozone profile from the surface until 500 hPa for 28/09/2019.

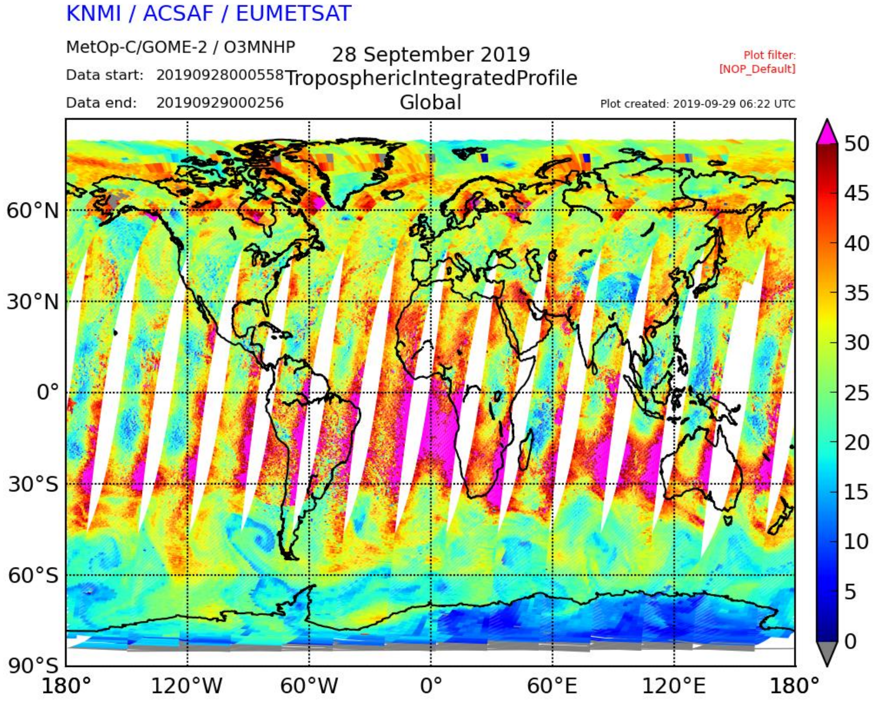


Figure 10: Vertical integrated ozone profile from the surface until the tropopause for 28/09/2019.

As an illustration, also some examples are shown for GOME-2B for both products on 28/09/2019 (Figure 11 and Figure 12).

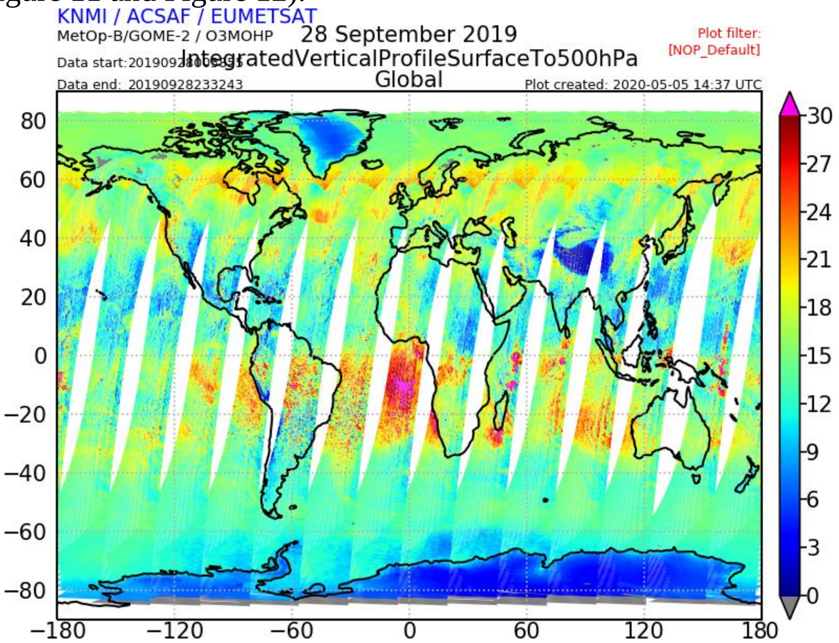


Figure 11: Vertical integrated ozone profile from the surface until 500 hPa for 28/09/2019 on MetOp-B.

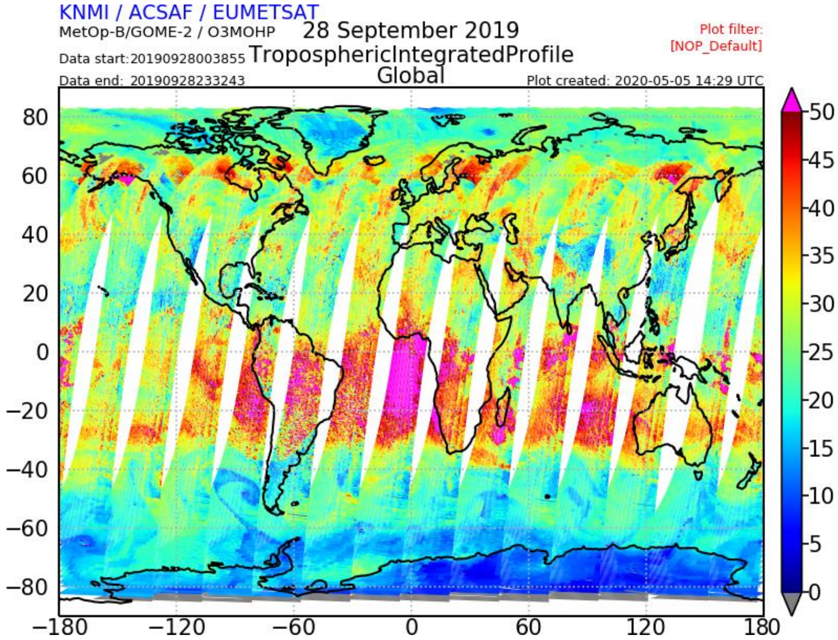


Figure 12: Vertical integrated ozone profile from the surface until the tropopause for 28/09/2019.

6. Conclusions

After comparing both methods, it is illustrated that the "fixed altitude method" shows *better* statistics. This can be easily explained by the exclusion of the influence of stratospheric ozone in the TrOC product, since we only take into account the ozone concentrations in the lower troposphere.

The comparison between the relative difference plots for both products shows that the amplitude in the seasonal cycle signal is also more pronounced in the tropopause related TrOC product, which results in the presence of more scatter in these plots (Figure 4 and Figure 7). Also the standard deviation is therefore more elevated in the tropopause related TrOC product.

It can be concluded that both products meet the user requirements.

Since there is a significant scan angle dependency present in the data, we would recommend the user to only consider the center pixels (nrs 9 – 16) in this operational version of the product. After a degradation correction update, the product should be available again for the end user for the full swath. This will be communicated through the operations reports, available on the website of the AC SAF (https:www.acsaf.org).

7. Acknowledgement

The ozonesonde data was made available by WOUDC (http://www.woudc.org), the SHADOZ network (http://croc.gsfc.nasa.gov/shadoz/) and the NILU's Atmospheric Database for Interactive Retrieval (NADIR) at Norsk Institutt for Luftforskning (NILU) (http://www.nilu.no/nadir/).

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