TORMS : TOTAL OZONE RETRIEVAL FROM MERIS IN VIEW OF APPLICATION TO SENTINEL-3

Dominique JOLIVET(1), Marc BOUVET(2), Christophe LEROT(3), Michel van ROOZENDAEL(3) and Didier RAMON(1)

(1) HYGEOS, EURATECHNOLOGIES, 165 Av de Bretagne, 59 000 Lille, France
(2) ESA/ESTEC, Wave Interaction & Propagation Section (TEC-EEP), Keplerlaan 1, PB 299, NL-2200 AG, Noordwijk, The Netherlands
(3) Royal Belgian Institute for Space Aeronomy (BIRA-IASB), Avenue Circulaire, 3, B-1180 Brussels, Belgium

Abstract

An algorithm has been developed to retrieve total column of ozone (TCO) using MERIS TOA reflectances, which include the ozone Chappuis bands. The method assumes that the TOA reflectance spectrum in the absence of gaseous absorption can be modelled by a third order polynomial. TCO is then retrieved by making use of the difference between this polynomial calculated from bands number 1, 2, 10, 12 and 13, and the measured reflectance in band number 3, 4, 5, 6, 7 and 8 where ozone absorbs.
This method has been applied to the full MERIS archive and MERIS TCOs have been compared to those retrieved more classically from the UV nadir sensor GOME-2A. The method is valid over bright and spectrally white surface such as snow/ice surfaces and optically thick clouds. The TCOs from MERIS and GOME-2A agree generally well over Antarctica, while MERIS tends to underestimate TCOs elsewhere. MERIS TCOs have also been compared to ground measurements and show a good correlation (bias and root mean square error of about 4 and 20 DU, respectively).

1. Introduction

The depletion of stratospheric ozone due to anthropogenic emissions of long-lived substances containing chlorine and other halogens was first identified as a matter of international concern in the mid-1970s and has received increasing attention since the mid-1980s after the discovery of the ozone hole. Today, in spite of the successful application of the Montreal Protocol and its amendments, the atmospheric halogen loading is still above natural levels and might remain so until the middle of this century. Monitoring of stratospheric ozone therefore remains extremely important, as the ozone layer has yet to recover from the atmospheric halogen loading caused by human action. Moreover, climate change also has an influence on stratospheric ozone while evidences that changing tropospheric ozone levels impact climate are becoming increasingly clear.

Reference space measurements of the total ozone column (TCO) are generally performed using the backscattered Earth radiation in the UV spectral range, through exploitation of the strong ozone differential absorption features in the 315-340nm (Huggins bands). Current UV instruments generally provide daily global coverage at a spatial resolution of the order of several tens of kilometres, compatible with the typical scales of the ozone variability. Current state-of-the-art data products have an accuracy of the order of a few percent, and a long-term stability better than 1%/decade.

Primarily designed for land and ocean colour monitoring, MERIS is a multispectral imager covering the visible to near infrared part of the spectrum in a series of discrete spectral bands. Although they do not sample the UV part of the spectrum, MERIS channels are sensitive to ozone absorption in the visible Chappuis bands which extend from approximately 400 to 700 nm. Despite the fact that ozone absorption spectral features are generally difficult to disentangle from surface effects in this region, the potential to measure total ozone from MERIS observations in this spectral region is investigated in this study. Although the MERIS algorithm suffers from limitations in terms of its applicability outside bright and spectrally white surfaces, a reasonable accuracy is only achieved in these particular observational conditions, the derived products offer the prospect of ozone mapping at high spatial resolution in comparison to existing UV sensors (MERIS has a spatial resolution of 300 m over land and 1km globally).

2. Theoretical background

Figure 1 shows gaseous transmittances for the MERIS channels (listed in Table 1, which also includes the bands of OLCI/Sentinel-3) for a typical Air Force Geophysics Laboratory (AFGL, Anderson et al., 1986) mid-latitude summer vertical profile. Gaseous transmittances have been calculated from the ratio of the TOA reflectances from radiative transfer calculations with and without the gaseous absorption.
Erreur ! Source du renvoi introuvable. summarizes respectively the 15 bands of the MERIS instruments onboard ENVISAT and the 21 bands of the OLCI instrument onboard Sentinel-3. Absorption in band 11 is due to oxygen (O_2), whereas water vapour (H_2O) is responsible to absorption in bands 9, 14 and 15. Ozone absorption mainly affects bands 3 to 8, and the maximum absorption is in the spectral range 550-620 nm where it is generally around 5% for usual solar and

viewing geometry encountered with sensor on polar orbit. Others bands are marginally affected by ozone absorption but a residual ozone absorption effect is still measureable by MERIS – with transmittance higher than 99.5%- and must be taken into account if high accuracy retrieval of the TCO is aimed at.

MERIS band number	OLCI band number	Central Wavelength (in nm)
	1	400.
1	2	412.5
2	3	442.5
3	4	490.
4	5	510.
5	6	560.
6	7	620.
7	8	665.
	9	673.5
8	10	681.25
9	11	708.75
10	12	753.75
11	13	761.25
	14	764.375
	15	767.5
12	16	778.75
13	17	865.
14	18	885.
15	19	900.
	20	940.
	21	1020.

Table 1 : MERIS and OLCI bands. In cyan are presented OLCI bands from MERIS heritage. In yellow are band only available on OLCI

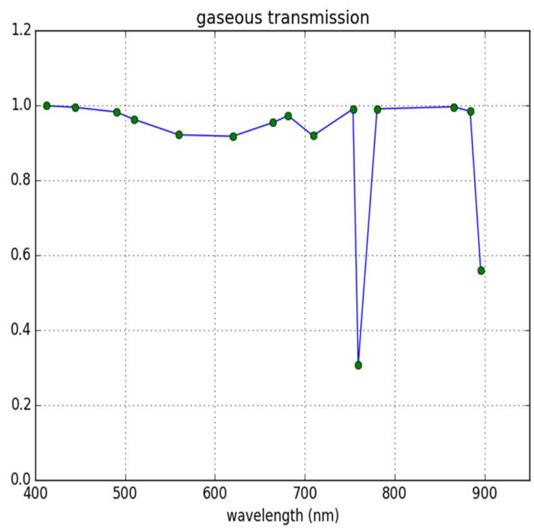


Figure 1 : Simulated gaseous transmittance in MERIS channels for a typical AFGL mid-latitude summer atmospheric profile (including water vapour and oxygen absorption) and a TCO of 300 DU. Underlying surface is a deciduous forest. Aerosol model is OPAC (Hess et al, 1998) maritime clean with an AOT of 0.1. SZA is 45°; VZA is 20° and RAA is 90°.

Table 2 summarizes the spectral ozone absorption through it optical thickness for 1000 DU.

MERIS Band number	Optical thickness for 1000 DU
1	0.00073
2	0.00407
3	0.02211
4	0.04381
5	0.10951
6	0.11252
7	0.05282
8	0.03695
9	0.02018
10	0.00992
11	0.00740
12	0.00811
13	0.00230
14	0.00135
15	0.00171

Table 2 : Ozone optical thickness for 1000 DU for MERIS bands convolving the Chehade et al. (2013) data at 243 K with the sensor spectral responses. For bands 1, 2, 10 12 and 13 (blue background), these values will be used to correct from ozone absorption

1.1. Inversion method

The method to retrieve the Total Column of Ozone (TCO) is based on the assumption that the MERIS absorption-free spectrum can be fitted by a simple polynomial fit on the observed target. Absorption-free channels are thus used to find the nominal fit. For ozone contaminated bands, the difference between observed and fitted values is used to retrieve ozone transmittances and therefore TCO.

	MERIS band number	OLCI band number
Free absorption bands used for nominal fit	1, 2, 10 ,12 and 13	1, 2, 3, 12, 16, 17 and 21
Bands affected by ozone absorption	3, 4, 5, 6, 7 and 8	4, 5, 6, 7, 8, 9 and 10
Bands excluded from the method	9 (H_2O), 11 (O_2), 14 and 15	11, 18, 19 and 20 (H_2O)

	(H_2O)	13, 14 and 15 (O_2)

Table 3: Selection of MERIS and OLCI bands for the TCO retrieval algorithm.

Bands contaminated by O_2 or H_2O are excluded from the process because of their high variability. Table 3 summarises MERIS and OLCI bands which can be used by the method.

Parameterization of the ozone transmittance

For bands significantly affected by ozone absorption, i.e., for bands 3, 4, 5, 6, 7 and 8, ozone transmittance will be calculated using accurate radiative transfer simulations for taking into account:

- Absorption-scattering coupling. Transmittances will be calculated every 25 DU for values between 25 and 600 DU and will be stored within Look-Up Tables (LUTs).
- Spherical shell atmosphere

For bands poorly contaminated by ozone absorption (band 1, 2, 10; 12 and 13), ozone transmittances will be approximated and calculated using **Erreur ! Source du renvoi introuvable.** and pre-calculated ozone optical thickness versus TCO (see **Erreur ! Source du renvoi introuvable.**). For these bands, accurate values are not absolutely needed.

$$T_{O3}(\theta, TCO, \lambda) = \exp(-\tau_{O3} AM(\theta) TCO) \quad (1)$$

Where AM(θ) is the airmass. In a spherical atmosphere in it can be written as

$$AM(\theta) = \sqrt{\left(\frac{R_{O3}}{H_{O3}}.cos\theta\right)^2 + 2.\frac{R_{O3}}{H_{O3}} + 1} - \frac{R_{O3}}{H_{O3}}.cos\theta \quad (2)$$

Where R_{O3} is the height of the O_3 layer, H_{O3} is the geometrical thickness of the layer and θ is the zenith angle

TCO calculation

The algorithm to retrieve the TCO is an iterative process which follows the following steps:

(i) Calculation of useful parameters to define the domain of validity of the method:

a. SIG_RESIDU: the TOA reflectances ρ_{MERIS}^{TOA} spectrum in bands 1, 2, 3, 4, 5, 6, 7, 8, 10, 12 and 13 is fitted by a third order polynomial. SIG_RESIDU is the chi square difference between the TOA reflectances ρ_{MERIS}^{TOA} and the fitted values ρ_{fit}^{TOA}. Very large values of SIG_RESIDU indicates that the TOA spectrum is far away from a third order polynomial fit and that third order polynomial is expected not to fit the absorption free TOA reflectance spectrum. Very low values of SIG_RESIDU indicates that the TOA measured reflectance spectrum can be fitted with a good accuracy by a third order polynomial: the residual signal containing the ozone absorption signature being small and the ozone retrieval accuracy is also small. It can also be the case for low signal to noise ratio.

$$sig\_residu = {}^{1}/_{n_{bands}} \sqrt{\sum_{band\ i} \left[\rho_{fit}^{TOA}(i) - \rho_{MERIS}^{TOA}(i)\right]^2} \quad (3)$$

b. NDVI (MERIS Normalized Difference Vegetation Index) parameter to identify surface covered with vegetation for which the retrieval method is not applicable. More generally high values of NDVI will indicated absorption free TOA spectra that will be hardly fitted by a 3rd order polynomial.

$$NDVI = \frac{\left(\rho_{MERIS}^{TOA}(band\ 13) - \rho_{MERIS}^{TOA}(band\ 7)\right)}{\left(\rho_{MERIS}^{TOA}(band\ 13) + \rho_{MERIS}^{TOA}(band\ 7)\right)} \quad (4)$$

(ii) Reflectances marginally affected by ozone absorption, in bands 1, 2, 10, 12 and 13, are corrected from the residual absorption ozone absorption using (1). The absorption free TOA spectrum obtained is then fitted by a third order polynomial.

(iii) The third order polynomial is applied to bands all bands (except bands 9, 11, 14 and 15) to obtain ρ_{pol}^{TOA}

(iv) Calculation of the chi square between the third order polynomial fit ρ_{pol}^{TOA} attenuated by the calculated ozone transmittance and the measured TOA spectrum ρ_{MERIS}^{TOA}. The TCO is retrieved by minimizing this chi square difference versus values of TCO.

(v) Finally, the estimation of the retrieval accuracy is assessed by calculated the fitting error estimate epsilon_fitting:

$$epsilon\_fitting = \frac{1}{n_{bands}} \times DIFF \quad (5)$$

Where

$$DIFF = \frac{\sqrt{\sum_{band\ i}\left[\frac{\rho_{pol}^{TOA}(i)T_{O3}(i)-\rho_{MERIS}^{TOA}(i)}{\rho_{MERIS}^{TOA}(i)}\times 100\right]}}{\max(1-T_{O3}(i))} \quad (6)$$

3. Domain of applicability and Validation against ground-based measurements

The MERIS TCO product has been compared with ground-based measurements. Total ozone is measured from ground by different types of instruments: UV spectrophotometers such as the Dobson and Brewer instruments on one hand, and UV-Visible DOAS spectrometers on the other. The required data sets are routinely archived in the World Ozone and Ultraviolet Radiation Data Centre (WOUDC - http://www.woudc.org),) and in the Data Host Facility (DHF) of the Network for the Detection of Atmospheric Composition Change (NDACC).

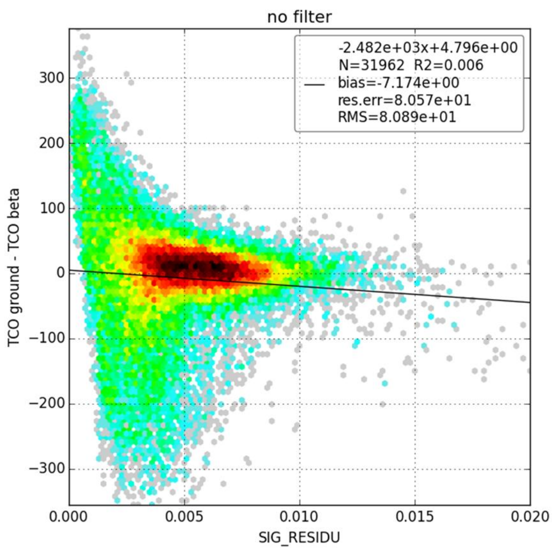


Figure 2 : Difference between ground TCO and MERIS TCO versus SIG_RESIDU

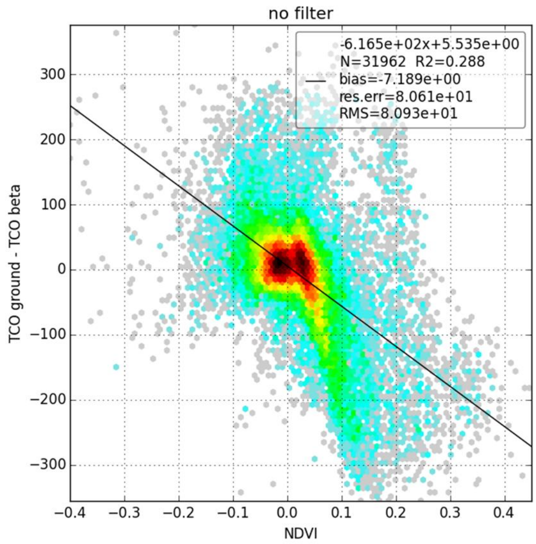


Figure 3 : same as Figure 2 but versus the NDVI

Figure 2 to Figure 5 show the comparison between MERIS TCO and ground based measurements of TCO from more than 20 stations for the whole MERIS mission (2002-2012) as a function of different parameters.

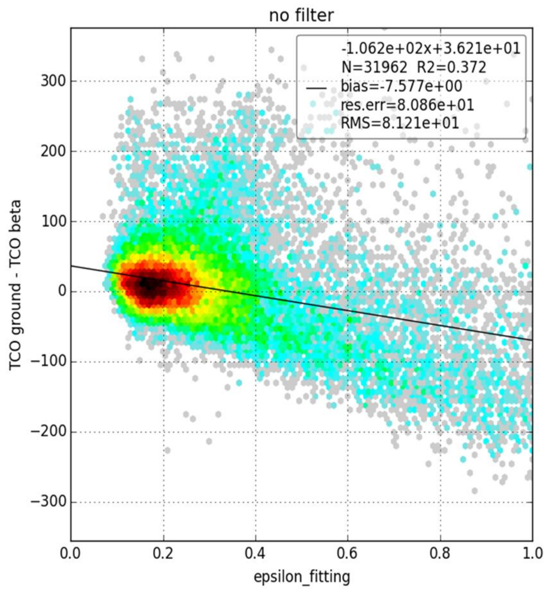


Figure 4 : same as Figure 2 but versus epsilon_fitting

The variation of the difference for all the match-ups between TCO and stations measurements as a function of these 4 parameters is shown in Figure 3. Higher discrepancies are obtained for small values of SIG_RESIDU, typically smaller than 0.003. High values of NDVI, from vegetation covered surfaces, lead to particularly large differences in TCO with ground measurements. The differences between ground measurements and MERIS retrievals are also correlated to the values of epsilon_fitting and it also appears that the retrieval is accurate only for high values of the TOA reflectance at 865 nm (band 13).

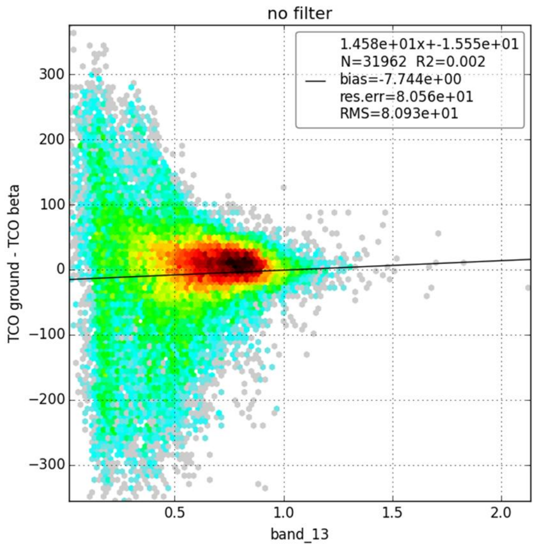


Figure 5 : same as Figure 2 but for the value of the TOA reflectance at 865 nm (band 13)

These four parameters can be considered as key parameters for the definition of the quality and the accuracy of the TCO product. From these results the domain of applicability of the TCO retrieval can be defined using threshold on the key parameters:

(i) SIG_RESIDU must be greater than 0.003
(ii) Reflectance at 865 nm must be greater than 0.8
(iii) NDVI must be smaller than 0.02
(iv) And epsilon_fitting must be smaller than 0.25

Applying these criteria to define the domain of applicability of the TCO retrieval algorithm and select matchups, the comparison between MERIS TCO and ground based measurements shows a good agreements as shown in Figure 6

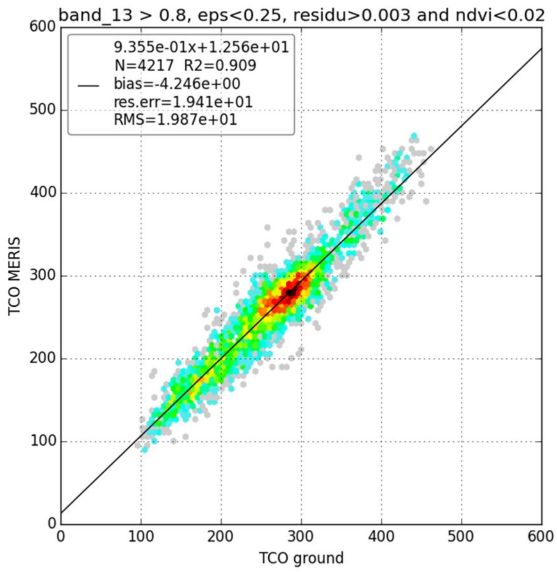
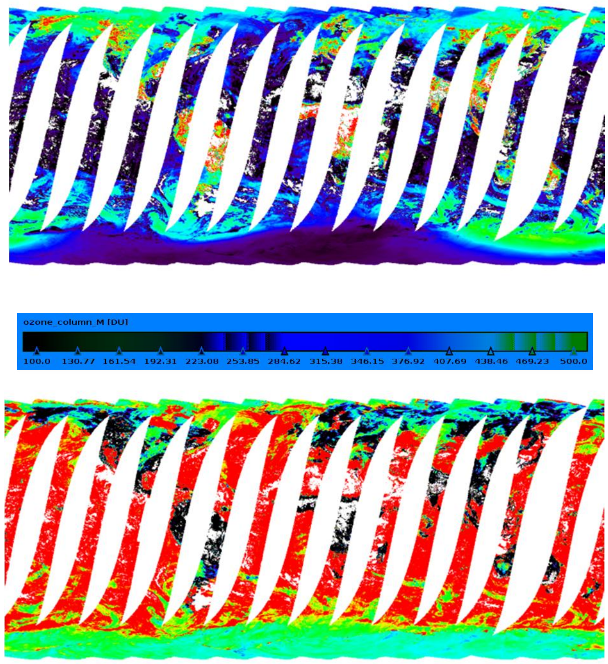


Figure 6: MERIS retrieved TCO versus TCO measured from 26 stations ground stations (in Dobson Unit). All MERIS pixels co-located with the ground-stations over the full mission (2002-2012) and for which the selection criteria are below the defined thresholds (see text) have been considered in this comparison.

4. Intercomparison

Classical methods to retrieve TCO are based on an analysis of the differential ozone absorption signal that can be detected in the 315-340 nm region in spectra of the earthshine backscattered radiation measured from nadir-looking space instruments. The Differential Optical Absorption Spectroscopy (DOAS) technique has been widely used to derive total ozone columns from European UV/Vis nadir-looking sensors. The direct-fitting algorithm GODFIT (GOME-type Direct FITting) is continuously developed and is a highly accurate evolution of the DOAS technique, by making use of the full information available in the 325-335 nm fit interval. This algorithm is used within the ESA O3_CCI project to generate multi-sensor consistent level-2 total ozone data sets (Lerot et al., 2014) and has been applied to measurements from GOME, SCIAMACHY, GOME-2 and OMI UV-Vis nadir sensors. TOC data products from those sensors have been extensively validated with ground-based data. Differences with ground data lie generally within 1% in most regions and may increase up to 2-3 % in Polar Regions. The scatter of the differences is generally around ±2.5% and the long-term stability is also excellent with drifts less than 1%/decade. We compare here MERIS TOC to GOME-2 TOC, as the latter has an almost daily global coverage and a equator-crossing time close to that of MERIS. Figure 7 shows in the upper panel the TCO retrieved from the MERIS observations without any filtering for October, 15th, 2008.



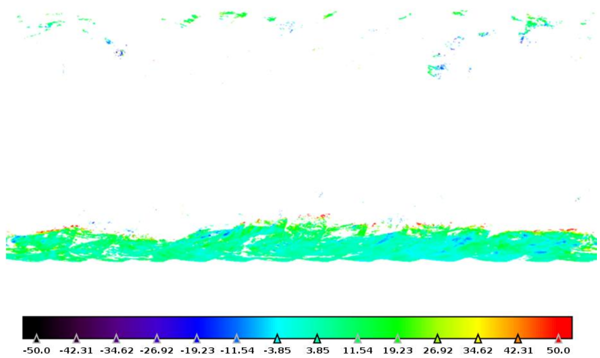
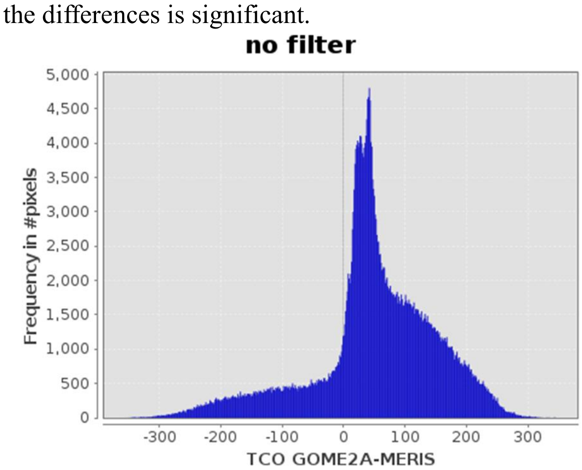


Figure 7: Top panel MERIS daily TCO for the 15 October 2008. No filter has been applied to the TCO product. Middle panel: Absolute TCO differences between MERIS and GOME-2A. Low panel: Same as middle panel but the product has been filtered with epsilon_fitting<0.25, ndvi<0.02, sig_residu>0.003 and band_13>0.8.

We see already that the MERIS TCOs are not physical in large parts of the world. For example, in Tropics, the MERIS TCOs are much too large over lands, while relatively homogeneous ozone fields are expected. This is even clearer when looking at the TOC MERIS-GOME-2A absolute differences (Figure 7- middle panel). The differences are generally very large, except over bright surfaces (snow/ice and clouds). This motivates an appropriate filtering of the MERIS product as discussed in the previous section. If the filters determined in the previous section are applied, the comparison becomes as illustrated in the bottom panel of Figure 7. The MERIS TOCs are generally in reasonable agreement with the GOME-2A TOCs.

Figure 8 shows distribution functions of the MERIS-GOME-2A TOC absolute differences for June, 15th 2008 without and with the defined filters. Without any filtering, huge differences are often observed and the distribution function is very wide and strongly asymmetric. When introducing the filters, the extreme differences and the distribution function gets closer to a Gaussian shape function. Note however that there is a large systematic low-bias in the MERIS TOC of about 20 DU compared to GOME-2A and that the scatter of the differences is significant.



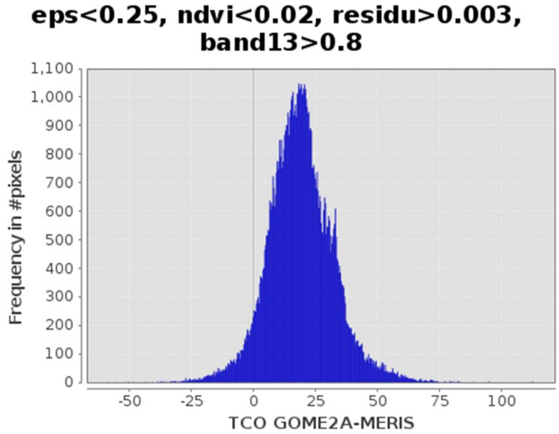
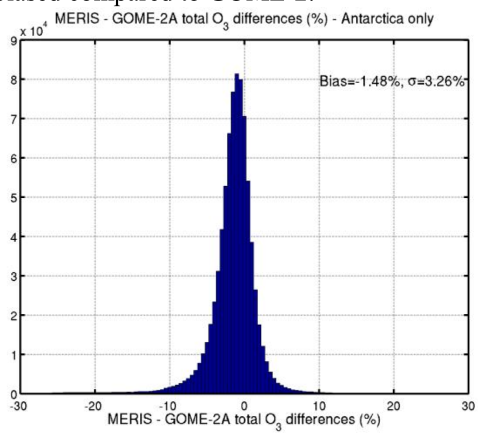


Figure 8: Histograms of the differences between daily TCOs from GOME-2A and MERIS without and with defined filters applied to the MERIS TCO product for the 15 June 2015.

In order to improve the statistics, MERIS TCOs have been compared to GOME-2 for 18 days distributed over the seasons in 2008. Figure 9 shows separately distributions of the MERIS-GOME-2 differences over and outside Antarctica as the algorithm seems to behave differently depending on the location. The two distributions are indeed significantly different. Over Antarctica, the distribution is characterized by a mean bias of 1.5% and a standard deviation of 3.3%, indicating a relatively good agreement with GOME-2. Outside of Antarctica, a larger mean bias of 4.4% is observed and the standard deviation of the distribution is 4.8%, which indicates that most MERIS TCO are low-biased compared to GOME-2.



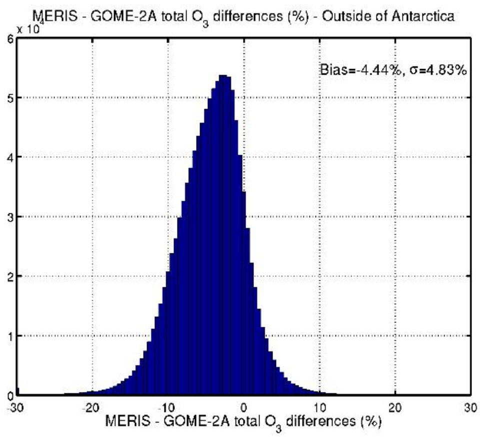


Figure 9: Histogram of the MERIS-GOME2 TCO relative differences for the 18 selected days. The upper panel shows the distribution for pixels over Antarctica and the bottom panel for pixels located elsewhere.

In order to better characterize the MERIS TCO product, dependences of the MERIS-GOME-2 differences with respect to a few key parameters have been investigated. The clearer dependence that we have identified is a dependence with respect to the ozone slant column SCD (i.e. the effective ozone column along the effective atmospheric light path). In reality, the ozone absorption signature in the measured spectra is linked to this so-called O_3 SCD, which can be estimated as the total ozone column multiplied by a geometrical air mass factor AMF. Here, we have estimated this AMF as 1+1/cos(SZA). Figure 10 illustrates the dependence of the MERIS-GOME2 differences with respect to the ozone SCD. For pixels out of Antarctica, a clear O_3 SCD dependence of the differences is visible, with MERIS TCO much too small for very low O3 SCDs and differences becoming smaller when the O3 SCD increases. Over Antarctica, if we exclude the first bin, a similar but smaller dependence is visible. This result suggests that the method for retrieving TCO from MERIS is accurate mainly when there is a strong O_3 signature in the radiances (combination of high SZA and high TCO).

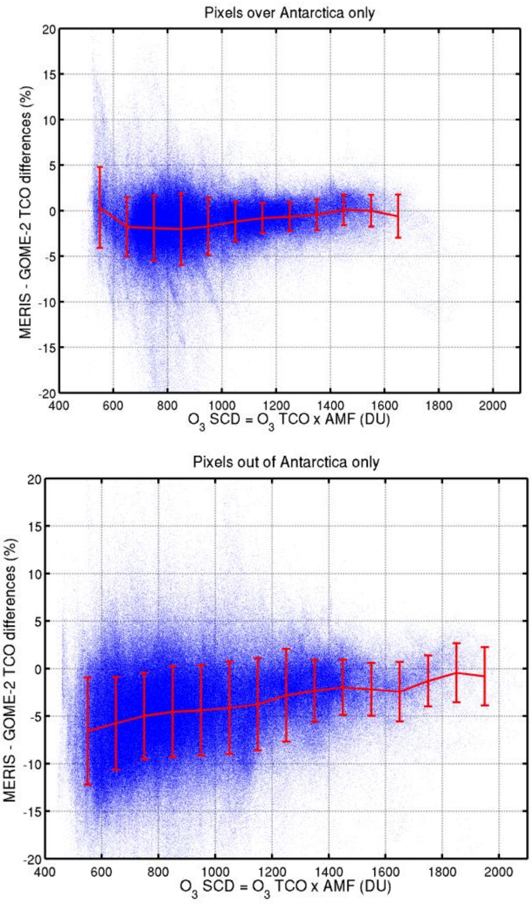


Figure 10: *O_3 slant column dependence of the MERIS-GOME2 TCO relative differences over (upper panel)or outside (bottom panel) of Antarctica. Blue dots correspond to individuals pixels and the red curve correspond to mean differences. The error bars represent the 2-sigma deviation.*

Figure 11 compares the O_3 gradient along longitude 135°E as seen by GOME-2 and MERIS for one day of the ozone hole season. The two instruments see consistent large scale spatial variation of the total ozone field. The high-frequency variations in the MERIS observations are roughly at the level of noise of the MERIS product (1-2%).

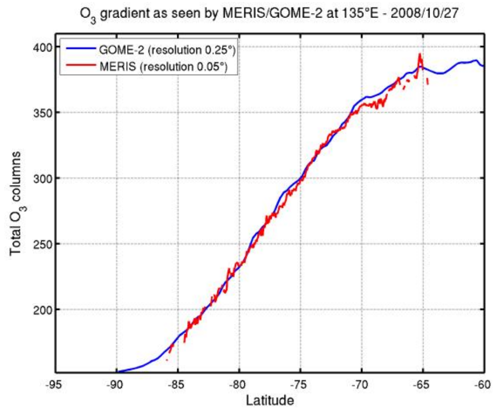


Figure 11: O_3 gradient in Southern Pole seen by MERIS and GOME-2A along the longitude 135°E for one day of the ozone hole season 2008.

5. Conclusion

An innovative algorithm has been developed for retrieving total ozone columns from MERIS observations. The algorithm relies on the exploitation of a series of ozone absorption bands in the visible. The measured reflectances at those bands are compared to an absorption free spectrum modelled by a 3rd order polynomial fitted through a series of bands not impacted by atmospheric absorbers. It has been shown that this algorithm provides total column ozone content with a reasonable accuracy only over bright surfaces as snow/ice or thick clouds. The product needs consequently to be properly filtered. A series of key selection criteria have been identified to apply such a filtering and associated thresholds identified to define the domain of validity of the MERIS TCO product. In particular, comparison of the retrieved MERIS TOCs with columns from ground-based observations and from reference UV nadir space sensors have contributed to this adjustment. Over Antarctica, the MERIS TOCs agree reasonably well with GOME-2 (mean bias=1.5%; standard deviation=3.3%), although MERIS might lead to too low columns in case of ozone hole conditions. Outside of Antarctica, the MERIS-GOME2 TOC differences are generally larger, and MERIS tends to lead to too low TOCs (mean bias=-4.4%; standard deviation=4.8%). It has been shown that the differences between the TOCs from MERIS and from the UV sensors are mostly dominated by the systematic component, especially out of Antarctica.

6. Reference

Anderson, G., Clough, S., Kneizys, F., Chetwynd, J., and Shettle, E.: AFGL atmospheric constituent profiles (0-120 km), Tech. Rep. AFGL-TR-86-0110, Air Force Geophys. Lab., Hanscom Air Force Base, Bedford, Mass., 1986.

Chehade, W., B. Gür, P. Spietz, V. Gorshelev, A. Serdyuchenko, J. P. Burrows, and M. Weber: Temperature dependent ozone absorption cross section spectra measured with the GOME-2 FM3 spectrometer and first application in satellite retrievals, Atmos. Meas. Tech., 6, 1623-1632, doi:10.5194/amt-6-1623-2013, 2013

Hess, M., Koepke, P., and Schult, I.: Optical Properties of Aerosols and Clouds: The Software Package OPAC, Bulletin of the American Meteorological Society, 79, 831–844, 1998.

Lerot, C., et al., 2014, Homogenized total ozone data records from the European sensors GOME/ERS-2, SCIAMACHY/Envisat and GOME-2/MetOp-A, J. Geophys. Res., 119, 3, 1639-1662*, doi:*10.1002/2013JD020831