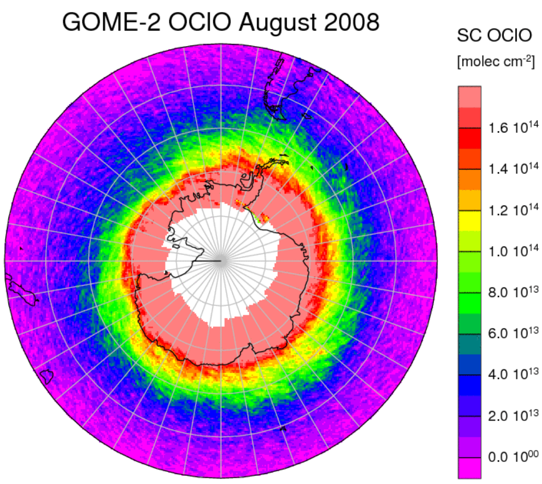
O3M SAF VALIDATION REPORT

Validated products:

Identifier	Name	Acronym
O3M-11	Offline Total OClO	OTO/OClO



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Reporting period: January 2008 – December 2008

Input data versions:	**GOME-2 L1b version 4.x**
Data processor versions:	**GDP 4.4, UPAS version 1.4.0**

Contents

ACRONYMS AND ABBREVIATIONS

CDOP	Continuous Development and Operations Proposal
DLR	German Aerospace Centre
DOAS	Differential Optical Absorption Spectroscopy
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
MetOp	Meteorological Operational satellite
NRT	Near-real-time
O3MSAF	Ozone Monitoring Satellite Application Facility
OMI	Ozone Monitoring Instrument
OTO/OClO	Offline Total OClO
SCIAMACHY	Scanning Imaging Spectrometer for atmospheric Chartography
SZA	Solar Zenith Angle

Applicable O3MSAF Documents

[ATBD] Algorithm Theoretical Basis Document for GOME-2 Total Column Products of Ozone, NO2, SO2, BrO, H2O, HCHO, OClO, tropospheric NO2 and Cloud Properties, DLR/GOME-2/ATBD/01, P. Valks, D. Loyola, N. Hao, M. Rix, S. Slijkhuis,.

[PUM] Product User Manual for GOME Total Columns of Ozone, NO2, SO2, BrO, H2O, HCHO, OClO, tropospheric NO2, and Cloud Properties, DLR/GOME/PUM/01, , D. Loyola, W. Zimmer, S. Kiemle, P. Valks, S. Emmadi.

[PRD] Product Requirements Document, SAF/O3M/FMI/RQ/PRD/001/Rev. 06, D. Hovila, J., S. Kiemle, O. Tuinder, H. Joench-Soerensen, F. Karcher, 2008.

Technical information

GOME-2 product name total column OClO (OTO/OClO)

Validation reporting period January 2008 - December 2008

Level-2 processor version GDP 4.4, UPAS version 1.4.0

Input GOME-2 Level-1B data version table

Start Date	Start Orbit	Level 1B Version
Jan 04, 2007	1093	4.0
Jan 07, 2009	11521	4.1.0
Apr 07, 2009	12796	4.2.0
Aug 18, 2009	14687	4.3.0

1. INTRODUCTION

Anthropogenic release of long-lived halogenated compounds into the atmosphere has lead to a significant increase of chlorine and bromine in the stratosphere, resulting in dramatic ozone loss in the polar winter stratosphere (ozone hole) and less spectacular but equally important loss at other latitudes. The stratospheric ozone layer acts as a protective shield against UV radiation from the sun, and reduction in stratospheric ozone amounts leads to increased UV radiation at the surface with impacts on the biosphere and human health. Therefore, emissions of long-lived chlorine and bromine containing substances have been regulated in the Montreal Protocol and its amendments, and atmospheric levels of the precursor substances have been decreasing over the last decade. In order to assess the effectiveness of the measures taken, in particular in the context of climate change which impacts on ozone recovery, monitoring of stratospheric chlorine and bromine contents is important.

Satellite instruments operating in the UV/visible part of the spectrum such as GOME, SCIAMACHY and OMI cannot observe the main chlorine reservoirs (HCl and $ClONO_2$), nor the main reactive chlorine substance (ClO). However, the OClO molecule which is thought to be formed mainly from the reaction of ClO and BrO has strong absorption features in the UV part of the spectrum, and OClO columns are routinely retrieved from satellite UV/vis measurements. As OClO is rapidly photolysed, it can only be observed at low sun around 90° solar zenith angle. The presence of OClO in the measurements is interpreted as indication for the presence of ClO which in turn is indicative of chlorine activation. Thus, OClO measurements can be used to identify chlorine activation and to monitor its change over time. Adding OClO slant columns to the operational GOME-2 data will extend the existing record of stratospheric chlorine activation measurements from 1995 to the future.

2. RETRIEVAL SETTINGS AND DATA SET USED

The results presented here are based on a one year data set of GOME-2 OClO columns for 2008. The IUP Bremen data are based on the consolidated lv1 data set version 4.0 until June 2008 and NRT lv1 data (also version 4.0) for the rest of the data. The operational data product OTO/OClO from DLR has been specifically produced for this intercomparison. In most of the figures, an older version of the product is being used which had a solar zenith angle cut-off if any of the solar zenith angles (satellite, top of atmosphere, bottom of atmosphere) was larger than 92° SZA. In the latest data version, this constraint has been removed and this is the data shown in the comparison with respect to solar zenith angle (Figure 14).

The DOAS retrieval settings used have been harmonised as much as possible between IUP Bremen and the operational data product OTO/OClO from DLR. They are listed in Table 1. Remaining differences between the two data products are linked to different treatment of spectral calibration, shift & squeeze and details of the interpolation and fitting routines.

For the SCIAMACHY data used in section 5, the same settings were used as for GOME-2 with four exceptions: 1) the SCIAMACHY-FM NO2 cross-sections were used, 2) the undersampling was calculated using the IUP-Bremen software, 3) an offset and slope were included in the fit based on the earth-shine, not the irradiance spectrum, and 4) a “magic ratio” spectrum derived from the ratio of two measurements taken with and without cloud is included in the retrieval.

Table 1: Summary of retrieval settings used

Parameter	Settings
Wavelength window	365 – 389 nm
Polynomial	5 coefficients
Background	Most recent solar irradiance
Cross-sections	
NO_2	GOME2-FM @ 223 K Gür et al., 2005
O_4	Hermans et al., 1999
OClO	Kromminga et al., 1999, 213 K, convoluted
Ring	GOMETRAN, provided by IUP-Bremen
Zeta	POL_ZETA.203 Version 1.2
Undersampling	Provided by DLR
Offset	1 / solar spectrum

3. CONSISTENCY OF GOME-2 OCLO PRODUCT

As a first step, the GOME-2 OClO data from the operational product are analysed for their internal consistency. For OClO, the expectation is that no OClO is retrieved under any conditions outside the activated polar vortex in spring. If present, OClO is situated in the stratosphere and surface elevation, surface spectral reflectance and clouds should not have an impact on the results. As no OClO is expected outside the vortex, light path differences (airmass factor variations) cannot play a role there and consequently, there should be no variation with solar zenith angle (SZA) or viewing angle.

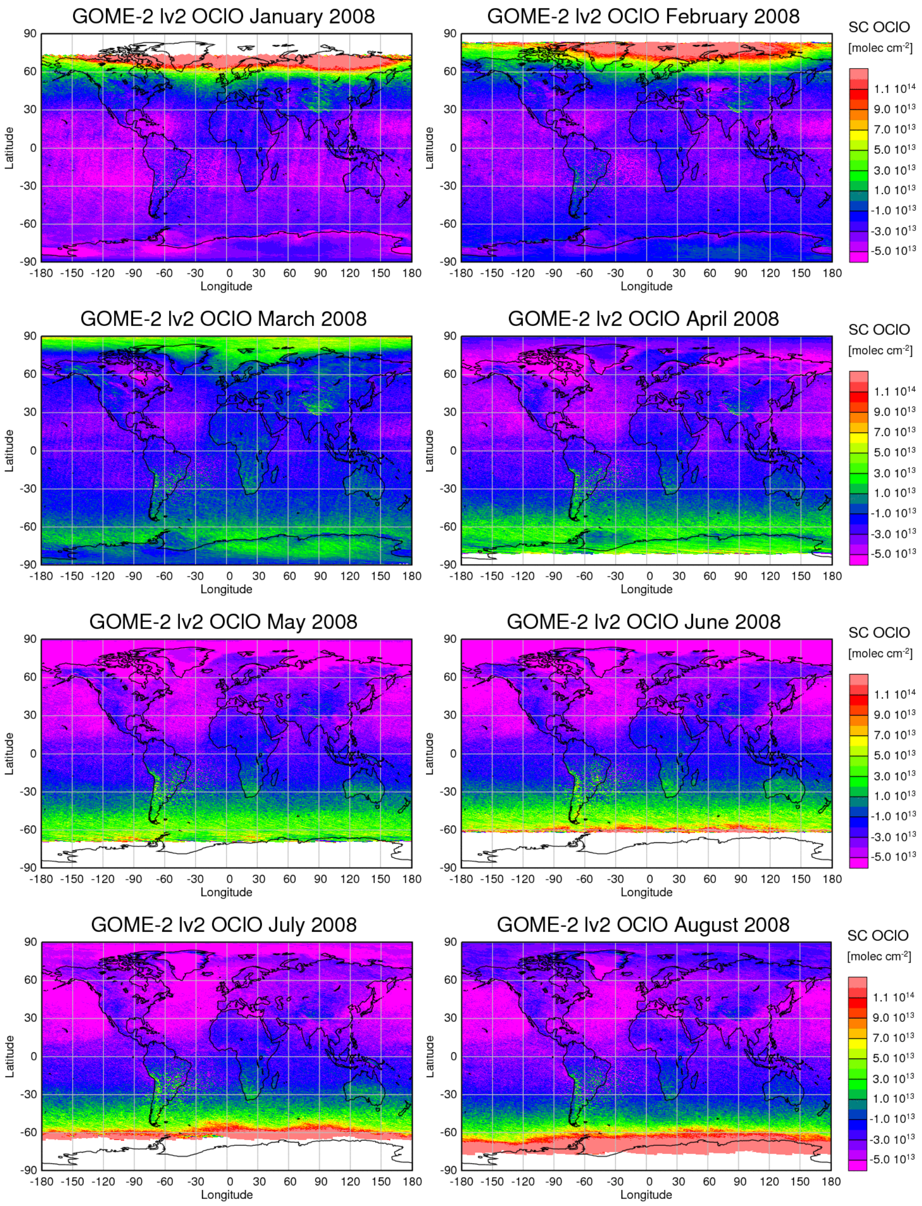
3.1 Overall pattern

In Figure 1, the monthly averages of the OClO slant columns from the operational products are shown for the year 2008. The colour scale used includes negative values to better display the range of values obtained. However, even using this scale, on some months values are outside the range.

GOME-2 OClO columns nicely pick up enhanced OClO in the periods of chlorine activation in the Northern Hemisphere (January and February) as well as in the Southern Hemisphere (July to September). However, the columns are not 0 outside these special regions as one would expect from atmospheric chemistry considerations. In particular in the Northern Hemisphere in summer, but also in Southern Hemispheric summer, very low values (-5×10^{13} molec cm^{-2} and less) are observed over large regions. These results are clearly unphysical. In addition, high values ($>2 \times 10^{13}$ molec cm^{-2}) are retrieved at high latitudes outside the regions where chlorine activation is expected. This poses a serious problem for interpretation of the data as these values would be taken for chlorine activation but probably are related to retrieval or lv1 problems.

Some of the patterns visible in the maps appear to be linked to topography (higher values over high mountains), reflectivity (higher values over bright surfaces) and sea-land contrast. This is indication of either spectral interference by O_4, Ring effect or surface albedo or of lv1 data calibration issues, e.g. linked to signal strength.

In some months, stripes (January), an overall offset (March) or systematic patterns (September) are apparent in the monthly averages. These are probably linked to GOME-2 instrument changes and are discussed in more detail in section 3.2.


GOME-2 lv2 OClO January 2008
GOME-2 lv2 OClO February 2008
GOME-2 lv2 OClO March 2008
GOME-2 lv2 OClO April 2008
GOME-2 lv2 OClO May 2008
GOME-2 lv2 OClO June 2008
GOME-2 lv2 OClO July 2008
GOME-2 lv2 OClO August 2008
Latitude
Longitude
SC OClO
[molec cm-2]
1.1 10^14
9.0 10^13
7.0 10^13
5.0 10^13
3.0 10^13
1.0 10^13
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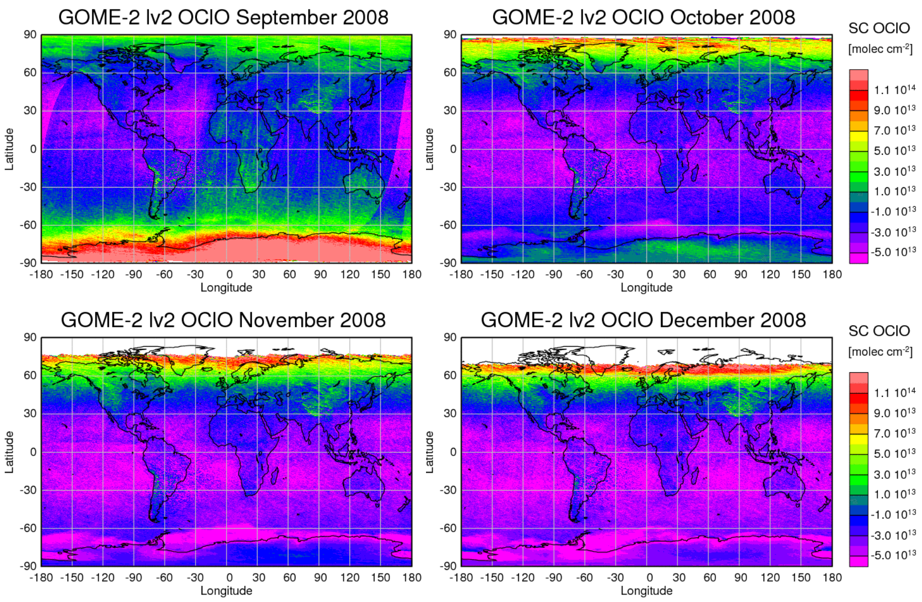


Figure 1: Monthly averages of OClO slant columns from the operational product for 2008

3.2 Lv1 problems

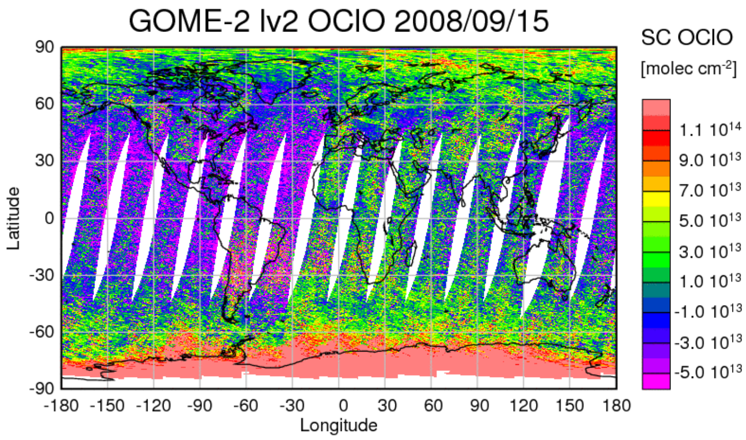


Figure 2: One day of OClO slant columns from the operational product showing the change in offset occurring when the solar spectrum changes

As could already be seen in Figure 1 for September, the OClO columns sometimes have large offsets to their "normal" values, probably as result of lv1 calibration problems. This is further illustrated in Figure 2, where results from a single day (September 15, 2008) are shown. Clearly, there is an offset in a group of orbits, and a similar pattern is observed on other days in September and in other months. In Figure 3, the values found close to the equator (+/- 20° latitude) are shown for each orbit in 2008 (some outliers have been removed). As one can see, there is a general low bias of several 10^{13} molec cm^{-2}, a smooth seasonal variation and several periods where a pattern of varying OClO offset is observed (January, march, twice in September). On the latter occasions, the daily images look as Figure 2. One explanation for this behaviour could be a slow drift in the lv1 which is occurring between the updates of the solar spectra which happens in the first orbit West of Europe. Such a drift can for example be explained by instrument switch-offs such as the double switch-off period occurring in September 2008. For this reason, instrument switch-offs are also indicated in Figure 3.

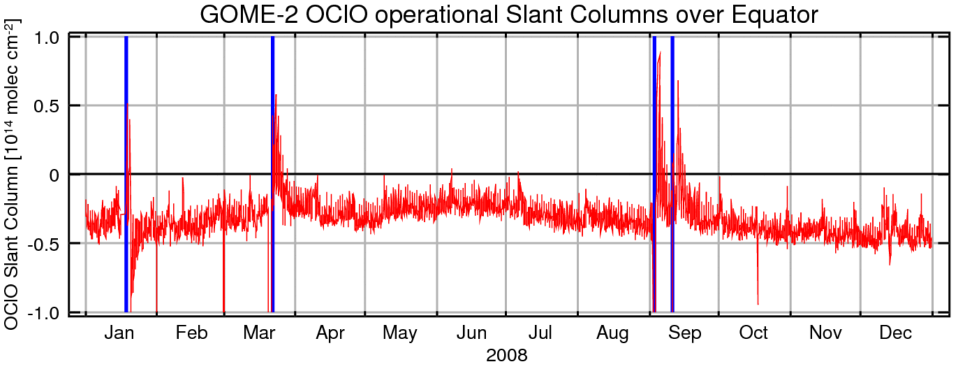


Figure 3: Evolution of GOME OClO operational slant columns in 2008. Horizontal lines indicate instrument switch-offs.

3.3 Random scatter

In the daily plot shown in Figure 2, the large scatter in the OClO columns is evident. A more quantitative estimate of the noise in the retrieved OClO columns can be gained by analysing the frequency distribution of values over a region where no OClO is expected to be present. This has been done in Figure 4 for data from May 2008. All measurements within the region (160° - 200° longitude, 20°S-20°N latitude) have been grouped in bins of 10^{12} molec cm^{-2}. As can be seen, the bias is about -3x10^{13} molec cm^{-2} compared to the expected value of 0. The distribution looks reasonably symmetric and Gaussian with a FWHM of about 10^{14} molec cm^{-2}. Considering the fact that OClO columns of 1x10^{14} molec cm-2 are indicative of strong chlorine activation, this has to be taken as large scatter. As will be shown in Figure 13, the scatter in SCIAMACHY data is about a factor of two smaller.

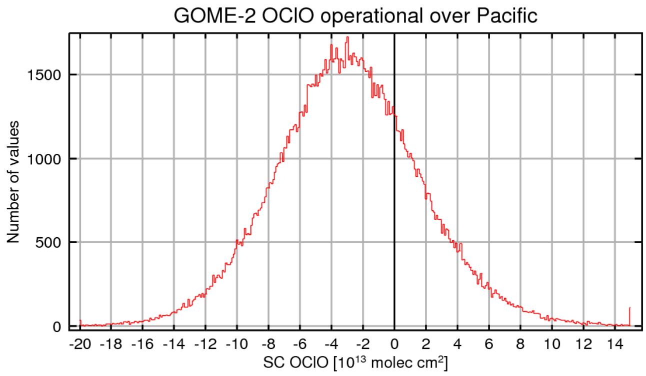


Figure 4: Frequency distribution of operational GOME-2 OClO columns over a region in the Pacific (160° - 200° longitude, 20°S – 20°N) for May 2008. Data are binned in intervals of 10^{12} molec cm^{-2}. Values outside the range displayed have been added to the two outermost bins.

A more realistic assessment of the scatter for OClO observations under polar vortex conditions would have to use data taken at low sun. There, intensities are lower but integration times are longer, partly compensating the increased noise. However, the simple assumption of absence of OClO might not always be correct under these conditions, and therefore, the equatorial scenario has been evaluated here.

3.4 Scan angle dependence

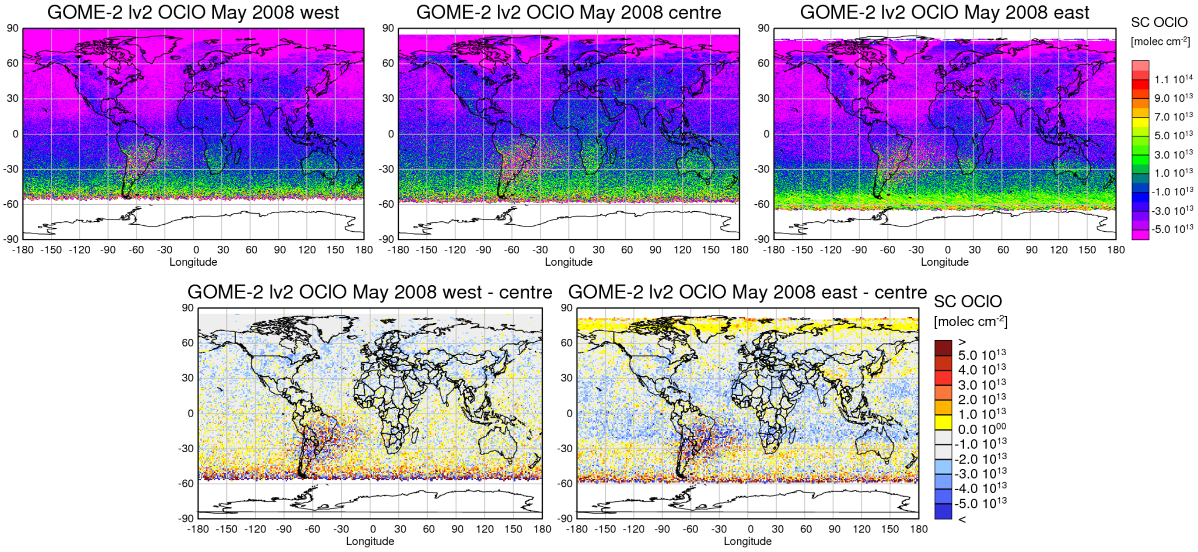


Figure 5: Comparison of operational OClO columns for May 2008 selecting different parts of the scan. In the lower panel, differences are shown. The differences have been binned on 1° x 1° for clarity.

In Figure 5, operational OClO columns are shown for three different subsections of the scan: west (1..8), centre (9..16), and east (17..24). As can be seen, the largest OClO columns are retrieved for the centre part of the scan and the smallest for the western part. The differences is very systematic and ranges from 0.6 10^{13} molec cm^{-2} at 40°S to 1.2 10^{13} molec cm^{-2} at 60°N. As no OClO is expected anywhere in May, this cannot be an airmass factor effect. Also, as it is more or less symmetric to the centre scan, it cannot be a solar zenith angle effect. The most probably explanation is an effect of the instrument viewing angle in the lv1 data.

3.5 Sensitivity to clouds

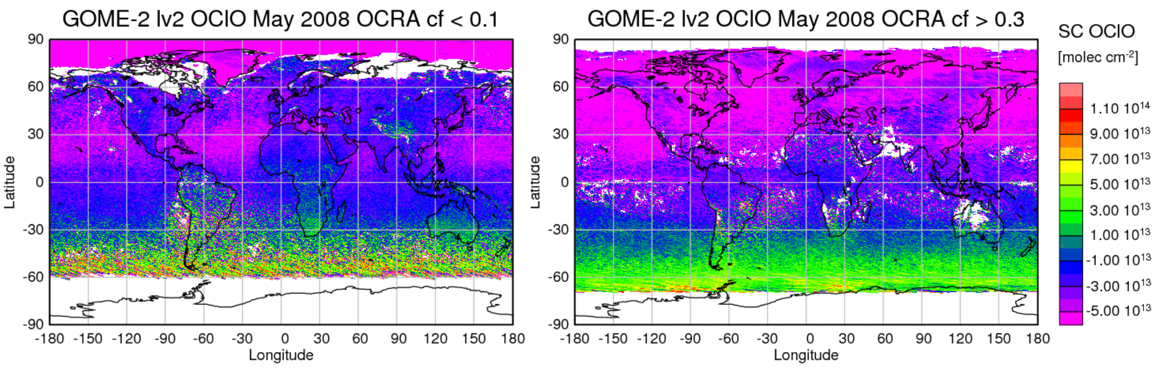


Figure 6: Comparison of GOME-2 operational OClO columns for May 2008 using only scenes flagged as having less than 10% cloud (left) and using those with more than 30% cloud fraction (right).

The sea-land contrast which is apparent in the monthly OClO averages suggests that clouds could have an impact on the retrieved values. As is illustrated in Figure 6 by comparing monthly averages using data with different OCRA cloud fraction thresholds for May 2008, this is indeed the case. In the Northern hemisphere, OClO columns retrieved in the presence of clouds tend to be lower by about 1-3 10^{13} molec cm^{-2}, in particular over continents. In the Southern Hemisphere, the effect is less pronounced, at least in May. This result indicates a retrieval problem either linked to bright scenes or to spectral interference from O_4 or Ring.

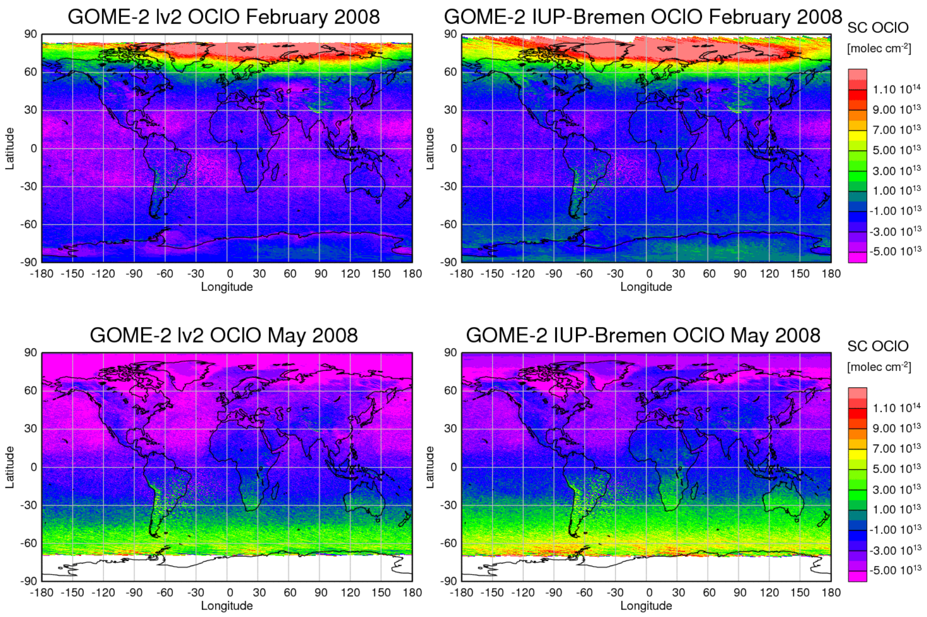
At high latitudes and over snow and ice, the current OCRA cloud fraction classification is probably not reliable as it is difficult to distinguish clouds from snow/ice. In these areas, scenes flagged as cloudy have significantly larger OClO columns.

4. VERIFICATION WITH IUP BREMEN GOME-2 PRODUCT

4.1 Overall comparison

In Figure 7, selected monthly averages of GOME-2 OClO are compared between the operational retrievals and the IUP-Bremen analysis. As can be seen, the overall pattern is very similar with the IUP-Bremen data having slightly larger values. In particular, the artefacts in the data which were discussed in section 3.1 are also present in the IUP-Bremen data. Therefore, this is not a problem of implementation but either of the retrieval settings (which were selected to be as similar as possible) or the lv1 data on which the analysis was performed.

One important difference between the two data sets is the cut-off value of the solar zenith angle. For the IUP-Bremen data, this is 92° at satellite while in the operational product it is 91° at top of atmosphere in the version shown here. As OClO is rapidly photolysed, this leads to higher OClO columns in the IUP-Bremen data set. In the latest operational product, the SZA cut-off has been relaxed.



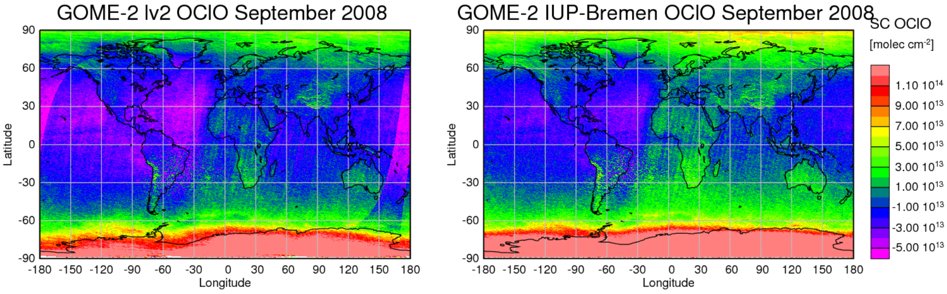


Figure 7: Comparison of selected months of GOME-2 OClO columns as retrieved by the operational processor (left) and the IUP-Bremen processor (right)

4.2 Comparison of individual orbits

While the monthly averages give a good overview on the consistency of the two data products, it is also interesting to compare individual orbits. Two randomly selected examples are shown in Figure 8 and Figure 9. As can be seen in both cases, the agreement is very good but not perfect, the operational data being slightly lower than the columns retrieved at IUP-Bremen. These results indicate that the implementation in the operational processor was successful, but some small differences remain. Unfortunately, the OClO retrieval proved to be very sensitive even to minor changes in the settings (such as for example the details of the undersampling correction used).

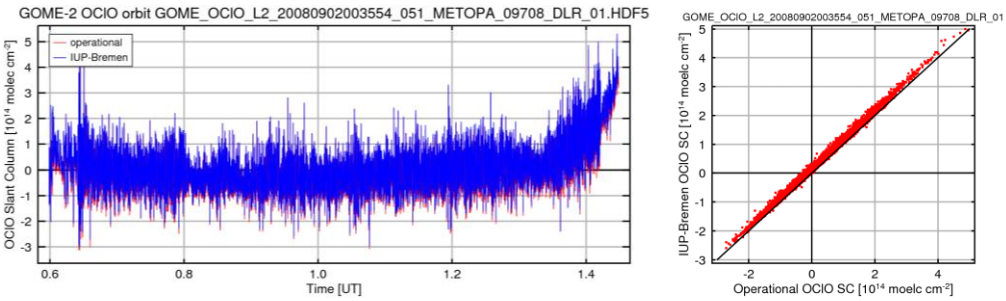


Figure 8: Comparison of one orbit of GOME-2 OClO data from the two processors in September 2008. The linear fit results in a slope of 1.013 and an offset of 1.23×10^{13} molec cm^{-2}. The correlation is 0.997.

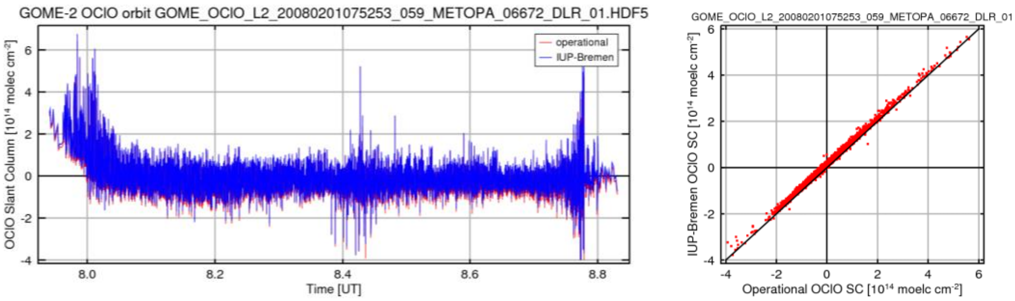


Figure 9: As Figure 8 but for an orbit in February 2008. The results of the linear fit are slope: 0.992, offset 1.19×10^{13} molec cm^{-2}, correlation 0.997.

5. COMPARISON WITH SCIAMACHY OCLO PRODUCT

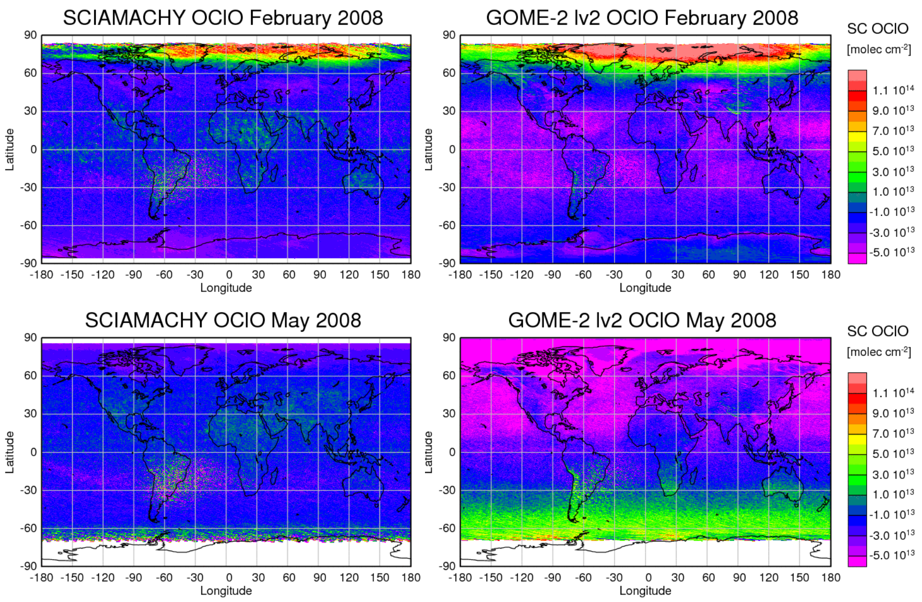
5.1 Overall comparison

In the absence of independent ground-based or airborne validation data for OClO, comparison with the results obtained from SCIAMACHY measurements is the best way to judge the overall quality of GOME-2 OClO columns. However, it should be kept in mind that the two instruments are very similar and the retrieval settings are kept as similar as possible, so that the two data sets cannot be seen as truly independent.

In Figure 10, four monthly averages of OClO from the two instruments are compared. As can be seen, the detection of chlorine activation in February and August 2008 is comparable in the two datasets, the GOME-2 data showing slightly larger areas of enhanced OClO and also higher values in the Northern Hemisphere. This could in part be the result of differences in overpass time and is discussed in more detail in the next section.

However, large differences exist in months where no OClO is expected, for example May and October. While in the SCIAMACHY data, all measurements are close to zero, this is not the case in GOME-2 data which show a large gradient in OClO with latitude with rather large values in one of the hemispheres. This problem which has already been highlighted before appears to be specific to the GOME-2 data.

At mid and low latitudes, similarities in the patters are observed between the two data sets (for example higher values over continents, lower values over the Antarctic sea ice), albeit with apparently larger amplitude in the GOME-2 data. These artefacts are then probably not related to instrumental problems but rather to retrieval issues.



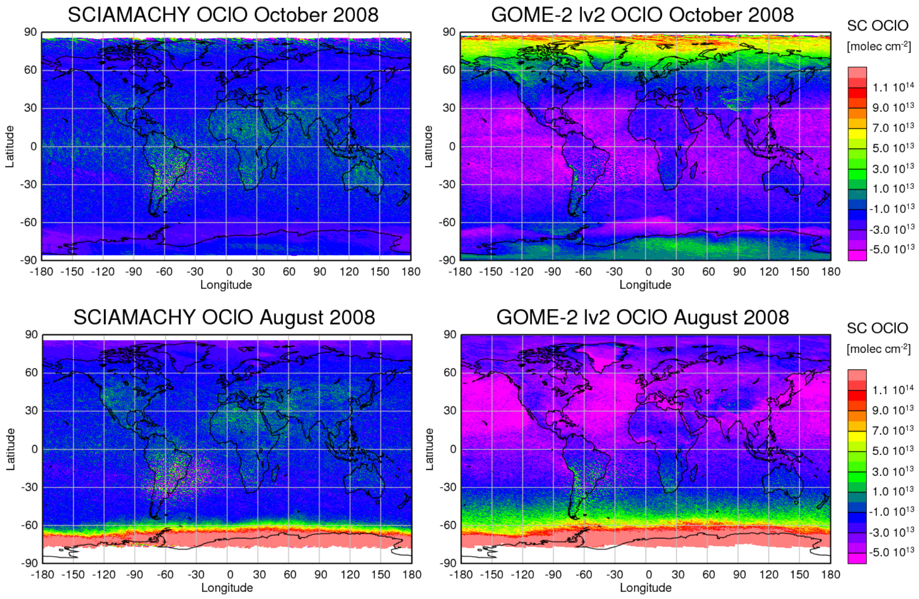


Figure 10: Comparison of selected months of SCIAMACHY OClO columns (left) with the corresponding operational GOME-2 data (right).

5.2 Comparison of scatter

In addition to the absolute columns, it is also interesting to compare the scatter in the OClO columns retrieved from measurements of the GOME-2 and SCIAMACHY instruments. This has been dome in two ways – by directly comparing the results for an individual orbit and by comparing the results of the analysis over the equatorial Pacific introduced in section 3.3.

One randomly selected orbit of GOME-2 and SCIAMACHY OClO columns is compared in Figure 11 and Figure 12. In the Antarctic polar vortex, chlorine was activated and enhanced OClO is observed in both data products. However, as can be seen in Figure 12, the scatter in GOME-2 data is much larger, in particular at larger SZA. Also, the GOME-2 slant columns show a curvature with latitude which is not observed in the SCIAMACHY results. South of about 70° SZA, GOME-2 data use longer integration times and the number of measurements is strongly reduced. These points are partly hidden below the SCIAMACHY values in the figure. This indicates that the large scatter in GOME-2 data is a signal to noise problem and not related to calibration issues.

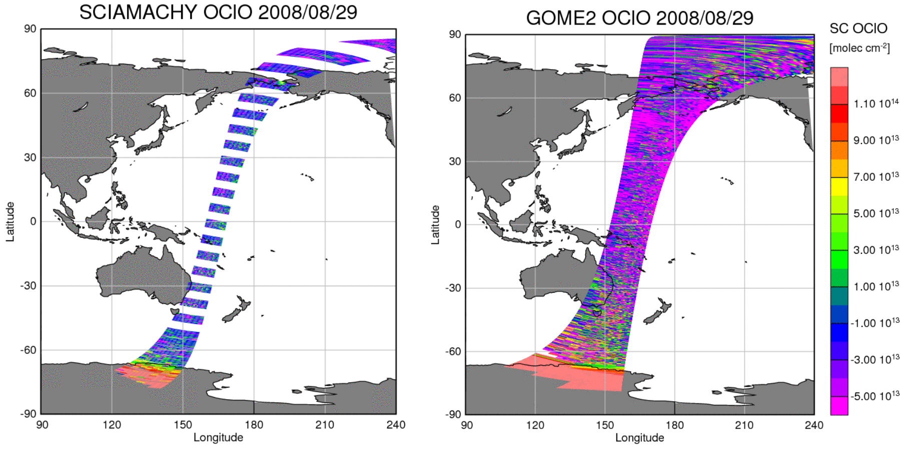


Figure 11: Comparison of one orbit of SCIAMACHY (left) and GOME-2 (right) OClO slant columns. The same data is compared in Figure 12.

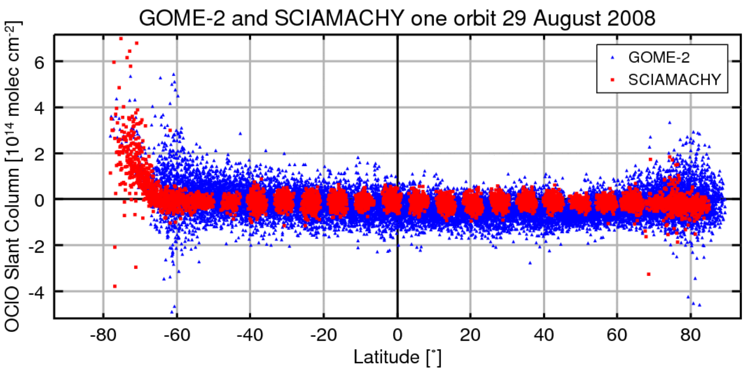


Figure 12: Direct comparison of the two orbits shown in Figure 11. Note that some enhanced GOME-2 OClO-columns are hidden below the SCIAMACHY points in the Southern Hemisphere.

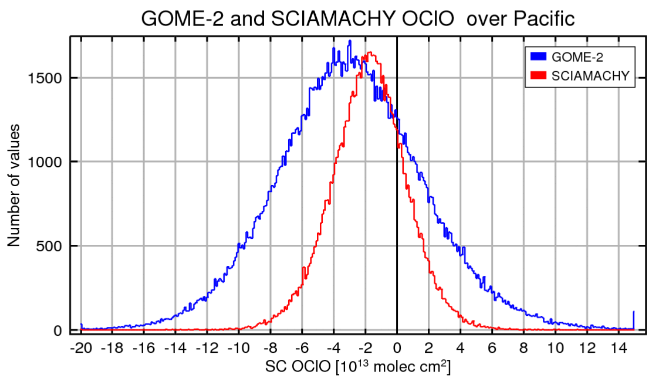


Figure 13: As Figure 4 but including IUP-Bremen OClO columns from SCIAMACHY. The latter curve has been scaled to have a similar maximum as the GOME-2 curve.

In Figure 13, the distribution of values over the equatorial Pacific is shown including both GOME-2 and SCIAMACHY results. The number of GOME-2 individual measurements is about three times as large as that of SCIAMACHY. Therefore, the SCIAMACHY curve has been scaled arbitrarily for clarity. As can be seen, the bias of the SCIAMACHY data is smaller (about 1.8×10^{13} molec cm^{-2}

and the FWHM of the distribution is 5x10^{13} molec cm^{-2}, about a factor of two smaller than that of the GOME-2 data. These numbers are consistent with the qualitative comparison shown in Figure 12.

When considering averaged values, the scatter in GOME-2 data is partly compensated by the larger number of measurements. As a rough approximation, the noise is larger by a factor of two which can be offset by averaging over four times as many measurements. As the number of data points per area is about three times larger for GOME-2 than for SCIAMACHY, the noise in monthly averages will be only slightly enhanced. However, at low sun where OClO measurements are most interesting, the GOME-2 data suffer from rapidly increasing noise and even using longer integration times (which is not done in SCIAMACHY), the scatter is large.

5.3 Comparison of SZA dependency

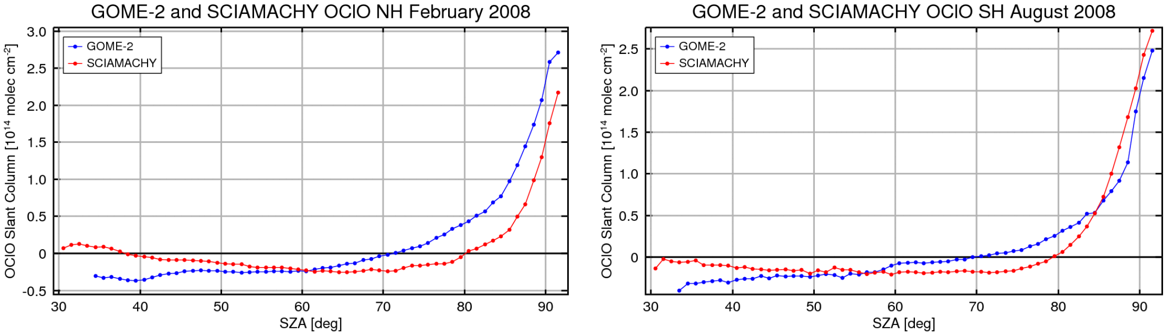


Figure 14: Comparison of SZA dependence of OClO columns from the operational GOME-2 product and the IUP Bremen SCIAMACHY data. Data from 20°W to 20°E are used. Left, data in the Northern Hemisphere are shown for February 2008; right, Southern Hemisphere data from August 2008.

As already mentioned above, the difference in overpass time of SCIAMACHY and GOME in combination with the rapid photolysis of OClO makes the direct comparison of data from the two instruments questionable. A better approach is to compare values taken at the same SZA as they should have probed OClO under similar photochemical situations. However, even this comparison is not perfect as measurements from the two instruments taken at the same SZA are over different latitudes. This is a problem at the edges of the polar vortex as usually the presence of OClO is limited to the region covered by the polar vortex, and comparing OClO measurements from inside and outside of the vortex makes no sense.

A further complication arises from the different spatial sampling of the two instruments. Firstly, SCIAMACHY has much poorer coverage than GOME-2 and therefore is more affected by spatial variability. This effect should not be systematic but result in increased variability. Secondly, the SCIAMACHY pixel size remains unchanged even at large SZA whereas GOME-2 pixels increase as the integration time is increased to improve the signal to noise ratio. As a result, different areas (and photochemical regimes) are covered by the two instruments even if the SZA at pixel centre is the same.

In Figure 14, OClO columns from GOME-2 and SCIAMACHY are compared as a function of SZA. All data within the longitude band of 20°W to 20°E was used, showing data from the Northern Hemisphere for February 2008 and Sothern Hemispheric data for August 2008. In this comparison, the latest operational OClO columns have been used which do not have an early SZA cut-off. The results confirm the conclusions already drawn from the comparison of the monthly maps: The SCIAMACHY data have a general negative bias and a rather steep increase of OClO with latitude at the edge of the activated polar vortex. In contrast, GOME-2 columns show a general increase with latitude with a rather smooth transition over the vortex edge. As one expects OClO to be mainly constrained to the vortex area, the GOME-2 results are less realistic than the SCIAMACHY data. There also is a difference in absolute values, GOME-2 columns being larger in the Northern Hemisphere and smaller in the Southern Hemisphere. This would still be the case if data were normalised to measurements at 70° latitude as was done in some studies using GOME-1 and SCIAMACHY data. As chlorine activation in the Antarctic vortex is expected to be more complete than in the Northern hemisphere, the SCIAMACHY results are more in line with expectations.

6. SUMMARY AND CONCLUSIONS

The GOME-2 OClO products OTO/OClO have been evaluated for internal consistency, agreement with the IUP Bremen GOME-2 products and with SCIAMACHY data. The main conclusions are

- Regions and periods of enhanced OClO in the polar vortices in both hemispheres are well represented in the OTO/OClO data.
- The agreement with the IUP Bremen OClO product used as template is not perfect but overall satisfying.
- There are many problems in the GOME-2 OClO data outside the regions of chlorine activation, leading to seasonal biases, sea-land contrast, cloud effects and scan angle dependencies. Some of the problems are known from other instruments (GOME-1, SCIAMACHY), pointing at retrieval issues. However, there also appears to be a lv1 data quality contribution.
- In comparison to SCIAMACHY (and GOME-1), the scatter of data is very large.

In summary, the implementation of the GOME-2 OClO slant column product into the operational processor was successful. However, as result of general problems in the OClO retrieval from GOME-2 measurements which are probably related to lv1 calibration issues, the product currently can mainly be used as qualitative indicator for chlorine activation and still has many artefacts. Further improvements in the data quality are needed to make the product fully adequate to extend the GOME and SCIAMACHY OClO data records.

Assessment of the absolute accuracy of the operational GOME-2 OTO/OClO product is difficult as truly independent validation data is not available. Comparison with collocated SCIAMACHY data show that differences can be as large as 5E13 molec cm^{-2} in monthly averages which is of the order of 30% of the absolute column in the activated polar vortex but much more under conditions where little or no OClO is expected. For individual measurements, the scatter is of the order of 5E13 molec cm^{-2} at low latitudes and 1E14 molec cm^{-2} at high latitudes at solar zenith angles with standard pixel size (80 x 40 km^2). Thus the random uncertainty of an individual measurement can be up to 100% (the target accuracy for OTO/OClO in the Product Requirements Document) in the activated vortex, is much less for pixels with longer integration time but even more at latitudes with little or no OClO.

7. OUTLOOK

Several open issues should be addressed in the near future to improve the OClO product:

- The zeta key data function used in the calibration of the lv1-data and as correction function in the fit was not yet straylight corrected. It is not expected that the updated lv1-data and zeta function will have a significant impact on the OClO fit but both should be tested as soon as updated lv1 data become available.
- In case of updates in the lv1 data product, the OClO retrieval should be evaluated on a smaller subset before operational delivery to investigate possible impacts on data quality
- Systematic analysis of residuals from a larger data set might help to identify the reason for the stronger SZA dependence of the GOME-2 OClO-product and might eventually lead to an empirical correction function that could be included in the fit as is the case in SCIAMACHY data

- The use of alternative OClO fitting windows should be investigated in more detail. So far, no better retrieval window could be found but this is a question of lv1 data version and more extensive tests might eventually lead to improved settings.
- Comparison with OClO products from OMI and also with GOME-2 scientific OClO retrievals from other groups might help to further improve the settings.

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