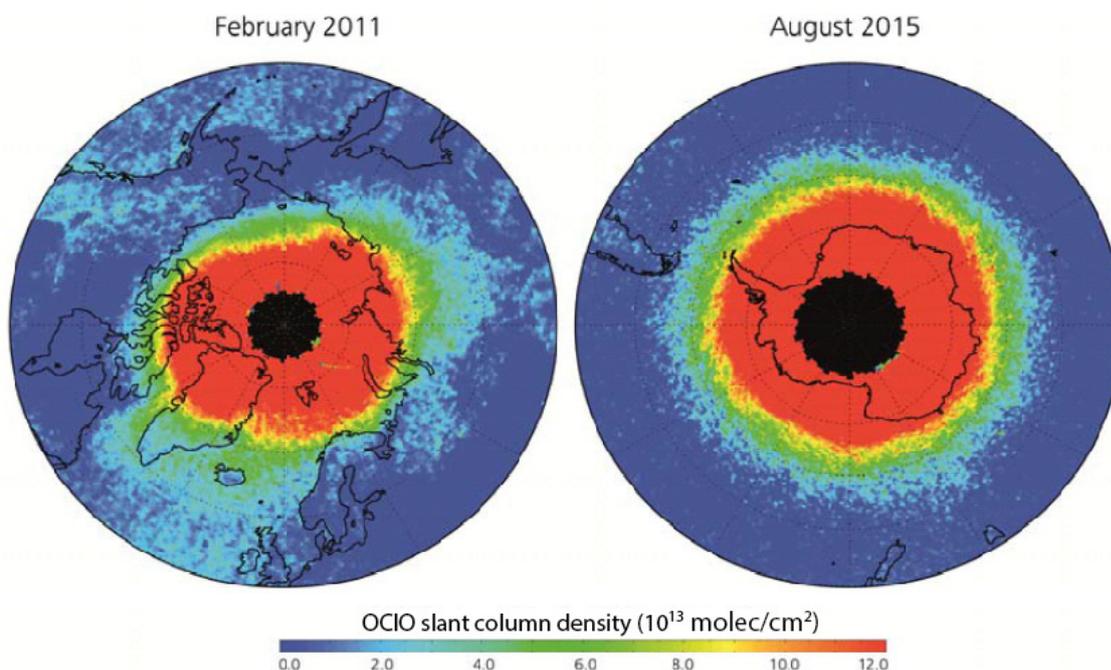


AC SAF VALIDATION REPORT

Validated products:

Identifier	Name	Acronym
O3M-119	OCIO Data Record from GOME-2A&B	MxG-RP1-OCIO

GOME-2MetOp [OCIO Slant Column](#)



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Ground-based data providers	BIRA-IASB, IUPB, IUPH, MPIC, INTA, NIWA, U. Toronto

external contributors / contributions externes au SAF

Teams contributing ground-based correlative measurements

Acronym	Organisation	Country
BIRA-IASB	Belgian Institute for Space Aeronomy	Belgium
IUP-Bremen	Institut für Umweltphysik, Universität Bremen	Germany
IUP-Heidelberg	Institut für Umweltphysik, Universität Heidelberg	Germany
MPIC	Max Planck Institute for Chemistry, Mainz	Germany
NIWA	National Institute of Water and Atmospheric Research	New Zealand
INTA	Instituto Nacional de Técnica Aeroespacial	Spain
UToronto	University of Toronto	Canada

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***Validation report of GOME-2 GDP 4.8
OCIO slant column
data record for MetOp-A and -B
DRR***

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ACRONYMS AND ABBREVIATIONS

AMF	Air Mass Factor, or optical enhancement factor
AC SAF	Atmospheric Composition Monitoring Satellite Application Facility
BIRA-IASB	Royal Belgian Institute for Space Aeronomy
DLR	German Aerospace Centre
DOAS	Differential Optical Absorption Spectroscopy
Envisat	Environmental Satellite
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
LOS	Line Of Sight
NDACC	Network for the Detection of Atmospheric Composition Change
NDSC	Network for the Detection of Stratospheric Change
O ₃	ozone
O3M SAF	Ozone and Atmospheric Chemistry Monitoring Satellite Application Facility
OCRA	Optical Cloud Recognition Algorithm
OMI	Ozone Monitoring Instrument
ROCINN	Retrieval of Cloud Information using Neural Networks
RRS	Rotational Raman Scattering
SCD	Slant Column Density
SCIAMACHY	Scanning Imaging Absorption spectroMeter for Atmospheric CHartography
SNR	Signal to Noise Ratio
SZA	Solar Zenith Angle
UPAS	Universal Processor for UV/VIS Atmospheric Spectrometers
UVVIS	ground-based DOAS ultraviolet-visible spectrometer
VCD	Vertical Column Density

DATA DISCLAIMER

In the framework of EUMETSAT's Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF, formerly O3M SAF), OCIO slant column data product is generated at DLR from MetOp-A and B GOME-2 measurements using the UPAS level-1-to-2 GDP 4.8 DOAS retrieval processor (see [ATBD] and [PUM]).

This report investigates the quality of the GOME-2A (2007-2016) and GOME-2B (2012-2016) OCIO GDP 4.8 slant columns datasets by comparing them to ground-based measurements at a selection of 8 DOAS zenith-sky stations around Arctic and Antarctic regions: Eureka (80°N), NyAlesund (79°N), Kiruna (68°N), Harestua (60°N), Marambio (64°S), Belgrano (78°S), Neumayer (71°S) and Arrival Heights (78°S). OCIO spectral analyses have been performed by each data provider using fixed noon spectra recorded at low SZA in the absence of chlorine activation. At each station, daily comparisons are performed by selecting satellite and ground-based SCD data pairs corresponding to similar SZA conditions, and by making the assumption that the AMF is similar for satellite and ground-based measurement in these geometries.

The following main conclusions can be drawn:

- Daily and monthly mean OCIO SCD time-series show that satellite and ground-based observations agree well at all stations, both in terms of seasonal and inter-annual variabilities.
- In the Southern Hemisphere, GOME-2A and B data have a tendency to underestimate ground-based observations by ~40%, while in the Northern Hemisphere the under-estimation is only of about 15%.
- Globally GOME-2B compares slightly better to the ground-based data than GOME-2A: when considering all the stations together, and only focusing on the activated period (July-August-September in the Southern Hemisphere and January-February-March in the Northern Hemisphere), the correlation coefficients derived from the daily scatterplots are about ~0.71 for GOME-2A and ~0.87 for GOME-2B, and the linear regression slopes are 0.58 for GOME-2A and 0.64 for GOME-2B.
- The results are within the user requirements as stated in the Product Requirements Document [PRD]: Threshold accuracy: 100%; Target accuracy: 50%; Optimal accuracy: 30%.

A. INTRODUCTION

A.1. Scope of this document

The present document reports on the verification and geophysical validation of the GOME-2 OCIO slant column data record produced by the GOME Data Processor (GDP) version 4.8 operated at DLR in the framework of the EUMETSAT Satellite Application Facility on Atmospheric Composition Monitoring (AC SAF). The aim is to investigate whether the GOME-2 OCIO slant column product fulfill the user requirements in terms of accuracy, as stated in the Product Requirements Document (PRD - Threshold accuracy: 100%; Target accuracy: 50%; Optimal: 30%).

A.2. Importance of OCIO

Anthropogenic release of long-lived halogenated compounds into the atmosphere has led to a significant increase of chlorine and bromine in the stratosphere, resulting e.g. in dramatic ozone loss in the polar spring stratosphere. Emissions of long-lived chlorine and bromine containing substances have been regulated since 1987 through 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 therefore of major importance. Satellite instruments operating in the UV/visible part of the spectrum such as GOME, SCIAMACHY and GOME-2 cannot observe the main chlorine reservoirs (HCl and ClONO₂), nor the main reactive chlorine species (ClO). However, the OCIO molecule, which is mainly formed through the reaction between ClO and BrO, has strong absorption features in the UV part of the spectrum. Although OCIO is only formed in sizeable quantities during the night, solar backscatter measurements of OCIO columns can be performed from space near the terminator where the efficiency of photolysis is reduced. This can be used to monitor the temporal evolution of the chlorine activation in both hemispheres, as demonstrated in the past using GOME and SCIAMACHY instruments (Wagner et al., 2001; 2002, Richter et al., 2005; Oetjen et al., 2011). Within the AC SAF, recent improvements based on a visiting scientist work at IUP-Bremen (Richter et al., 2015), have led to the creation of a reliable dataset of OCIO slant column densities (SCDs) for both GOME-2A and GOME-2B sensors. The implementation of these improved settings has been performed at DLR within the GDP 4.8 processor and this report addresses the quality of GOME-2A and GOME-2B data by comparing the satellite slant columns to correlative observations acquired by independent ground-based DOAS spectrometers in zenith-sky geometry.

A.3. Plan of this document

After presentation of the GOME-2 Data Disclaimer for OCIO column products, this document is divided into the following sections:

- A.** This introduction,
- B.** Validation protocol presenting the GOME-2, the reference data and the comparison method used,
- C.** Evaluation of the OCIO columns, by comparison with a set of 8 ground-based measurements
- D.** Conclusions
- E.** References

B. VALIDATION PROTOCOL

B.1. Data description

An improved OCIO retrieval algorithm for both GOME-2A and –B has been recently developed by Richter et al. (2015) within the framework of an O3M SAF Visiting Scientist project (VSA ID O3_AS14_02). With the improved DOAS algorithm described in Richter et al. (2015) and here below (Section B.1.1), the quality of the GOME-2 OCIO columns is clearly improved compared to the demonstrational results in the CDOP-1 (Richter et al., 2009). The demonstrational data were indeed affected by several problems outside the chlorine activated regions, leading to seasonal biases, sea-land contrast, cloud effects and scan angle dependencies (Richter et al., 2009). Some problems were related to retrieval issues, but also to Level 1 quality, leading to very large scatter in the data in comparison to SCIAMACHY (and GOME-1) retrievals.

B.1.1. GOME-2 OCIO retrieval: algorithm description

The operational GDP 4.8 OCIO retrieval algorithm for GOME-2 is fully described in the corresponding Algorithm Theoretical Basis Document [ATBD] and detailed information about the development of the analysis method can be found in Richter et al. (2015) visiting scientist report. The updated DOAS retrieval is performed in the UV wavelength range 345-389 nm to reduce bias and noise in the OCIO slant columns. The GOME-2 key data parameter Eta is fitted as another effective cross-section to correct for residual polarization errors in the level-1 product. This inclusion significantly improves the fitting residuals of the OCIO fit. Two empirical correction functions (derived from mean DOAS-fit residuals) are also included as additional (pseudo-) absorption cross-sections in the DOAS-fit: a mean residual and a scan angle correction function. These two empirical functions correct for positive off-sets and scan angle dependences in the OCIO columns. The details of the retrieval settings are synthesized in table B.1.

With this updated DOAS algorithm, the quality of the GOME-2 OCIO columns is clearly improved compared to the demonstrational results based on the original algorithm from 2009, especially for the GOME-2B instrument. However, an additional offset correction is needed to correct for remaining biases in the OCIO columns (e.g. non-zero OCIO columns over areas without chlorine activation), the temporal drifts observed mainly in the OCIO data from GOME-2A (see Richter et al., 2015). To that end, a simple normalization is applied on an orbital basis. The mean OCIO slant column for the area between 50°N and 50°S (a latitude region without chlorine activation) is determined for each GOME-2 orbit, which is then subtracted from the retrieved OCIO slant columns for the complete orbit.

Table B.1 DOAS settings used for the GOME-2 OCIO retrieval GDP 4.8.

Fitting interval	345-389 nm
Sun reference	Sun irradiance for GOME-2 L1 product
Wavelength calibration	Wavelength calibration of sun reference optimized by NLLS adjustment on convolved Chance and Kurucz (2010) solar lines atlas
Polynomial	4 th order, 5 coefficients
Offset	linear
Absorption cross-sections	
- NO ₂	Gur et al., 2005, 223K
- O ₃	Gur et al., 2005, 223K and 243K

- O ₂ -O ₂	Hermans et al., 1999
- OCIO	Kromminga et al., 2003 at 213K
- Ring effect	Vountas et al., 1998
- Key data	Eta
- Empirical functions	2: mean residual and scan angle correction

As OCIO photolyses rapidly, it can only be observed at large solar zenith angle and under these circumstances the calculation of an AMF and a vertical column is not trivial. It is complicated by rapid photolysis, the change in SZA along the line of sight, and also the uncertainty in the vertical profile (Richter et al., 2005; Oetjen et al., 2011). Therefore, as previous studies, the GOME-2 GDP data products only contain (corrected) OCIO slant columns. The OCIO SCD are mostly created by the BrO + ClO → Br + OCIO reaction (Solomon et al. 1987; Toumi 1994), and as the BrO concentrations vary only slightly, the formation of OCIO is limited by the ClO availability. OCIO SCD are thus a useful qualitative indicator of the chlorine activation (Sessler et al., 1995; Richter et al., 2005; Oetjen et al., 2011).

A flag, defined as in table B.2, indicates when valid (enhanced) OCIO column values can be expected from the GOME-2 data (OCIO_Flag set to 1 or 2).

Table B.2 OCIO flag definition (as in [PUM]).

Bit	Value	Description
0	1	Measurement (daylight) with large solar zenith angle ($85^\circ < \text{SZA} < 89^\circ$) Note: OCIO can only be observed at large solar zenith angles
1	2	Measurement during twilight ($89^\circ < \text{SZA} < 92^\circ$) Note: OCIO can only be observed at large solar zenith angles

B.1.2. Correlative ground-based datasets

OCIO columns have been retrieved from the ground since 1986 using Differential Optical Absorption Spectroscopy (DOAS) measurements in the Antarctic and Arctic (Solomon et al., 1987; Kreher et al., 1996; Gil et al., 1996; Richter et al., 1999; Tørnkvist et al., 2002; Vandaele et al., 2005; Friess et al., 2005).

For this study, stations situated above 60° latitude (north and south) have been selected (see table B.3 and figure B.1) and OCIO SCD data retrieved from different groups have been collected. It can be seen in figure B.2 that this dataset ensures a good temporal coverage, with stations measuring from one year (Marambio) to the whole Metop-A time length (Neumayer and Arrival Heights). A good coverage of the Arctic and Antarctic region is also assured, with half of the stations in the Northern Hemisphere and half in the Southern Hemisphere. However, as briefly described in Table B.4, the ensemble of ground-based dataset is an aggregate of existing measurements and there is no harmonization in the retrieval choices of the different group processing the OCIO data. Different wavelength regions for the OCIO analysis have been used by each group, depending on their instruments wavelength coverage and their sensitivity.

Table B.3 List of ground-based stations included in this study.

Station	Country	Lat [°]	Long [°]	Group/PI
Eureka	Canada	80.053	-86.416	UToronto, Kim

				Strong
NyAlesund	Norway/Svalbard	78.9	11.9	IUPB, Andreas Richter
Kiruna	Sweden	67.84	20.41	MPIC, Thomas Wagner
Harestua	Norway	60.22	10.75	BIRA, Michel Van Roozendaal
Marambio	Antartica	-64.266	-56.733	INTA, Margarita Yela González
Neumayer	Antartica	-70.62	-8.27	IUPH, Udo Friess
ArrivalHeights	Antartica	-77.83	166.65	IUPH, Udo Friess
ArrivalHeights	Antartica	-77.83	166.65	NIWA, Richard Querel
Belgrano	Antartica	-77.866	-34.616	INTA, Margarita Yela González

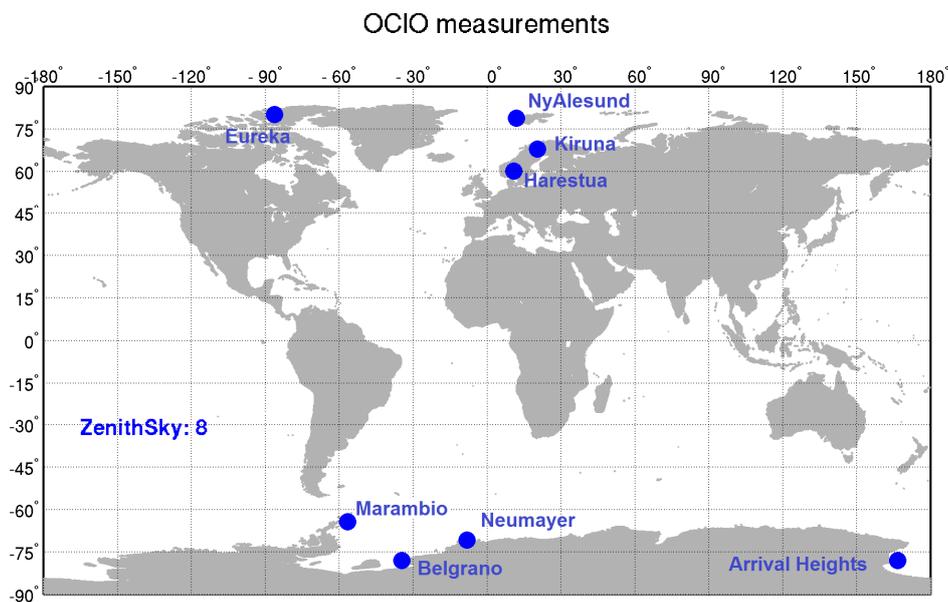


Figure B.1 Map of OCIO ground-based datasets used in this study.

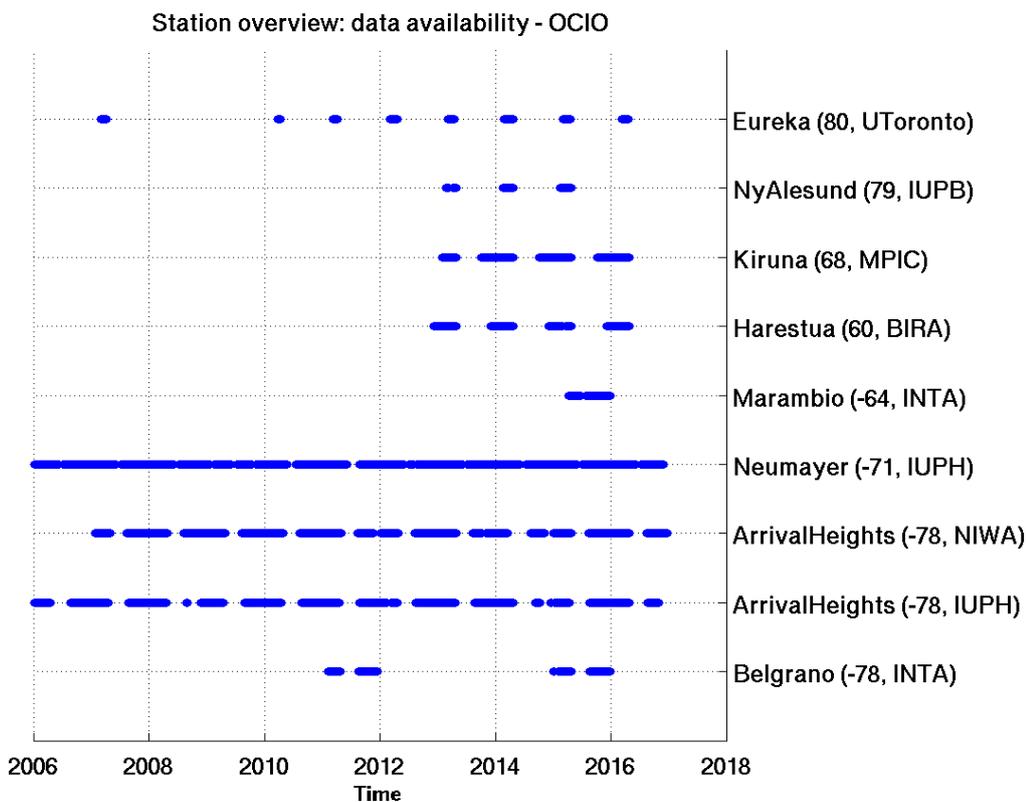


Figure B.2 Temporal coverage of the OCIO ground-based datasets used in this study.

Table B.4: Description of the different ground-based OCIO datasets used in this study.

Group Station	SCD range for OCIO analysis	Reference spectra	Cross-sections	Other info
BIRA Harestua	347-374nm	Fix reference outside activation period	Kromminga et al. 2003, 213K	
IUPH Arrival Heights and Neumayer [Friess et al., 2005]	364-391nm	spectra are analysed using fixed noon spectra at low SZA, when no OCIO can be expected	Kromminga OCIO cross section at 233 K	Data is filtered for SZA < 94° and RMS < 1e-3. The OCIO dSCD error is simply the 1-sigma fit error.

MPIC Kiruna	347,7-390 nm	a fixed reference recorded at the minimum SZA conditions in October or March (outside of polar vortex)	OCIO (Kromminga et al., 2003, 213K), O ₃ (Bogumil et al., 2003, 223 K), NO ₂ (Vandaele et al., 1997, 220K), O ₄ (Thalman et al., 1997, 273K), BrO (Wilmouth et al., 1999, 228K), Ring, Ring x lamda ⁴ .	
NIWA Arrival Heights [Kreher et al. 1996]	404-424nm	Fixed reference	Kromminga et al. 2003, 213K	AM and PM twilight, all SZA
IUPB NyAlesund	365-388.5nm	Fixed reference for each year	OCIO (Kromminga et al., 1999), NO ₂ (Vandaele et al., 1997, 220K), O ₄ (Hermans et al., 1999), Ring (Vountas et al. 1998)	
INTA Belgrano and Marambio	363-391nm	reference taken during the non-active period	OCIO (Kromminga et al., 2003, 213K), NO ₂ (Vandaele et al., 1997, 220K and 298K), O ₄ (Thalman et al., 1997, 273K), Ring (250K and 220K; Chance and Spurr, 1997)	
UToronto Eureka	350-380nm	not stable enough for a fixed reference, so daily references is used noon zenith spectrum averaged in a 0.03 degree SZA window	OCIO (204K, Wahner et al., 1987), NO ₂ (220 K, Vandaele et al., 1997), O ₃ (223 K, Bugomil et al., 2003), O ₄ (Hermans et al., 2003), BrO (223K, Fleischmann et al., 2004), Ring (Chance and Spurr, 1997)	Twilight spectra averaged in 0.5 degree SZA bins prior to QDOAS analysis

As described shortly in table B.4, the data of Eureka station was also a candidate for the comparison with GOME-2 data, but the ground-based data could not be analysed with a fixed reference spectra for the whole period due to instrumental instabilities, and the data are thus not suitable for the comparison to absolute OCIO SCD as measured by the satellite.

The statistical error in OCIO SCDs during twilight is on the order of 2×10^{13} molec/cm² (Friess et al., 2005) for Neumayer and Arrival Heights.

B.2. Comparison method

For the comparison, a method similar to Richter et al. (2015) and Oetjen et al. (2011) has been adopted. The GOME-2 GDP 4.8 OCIO SCD data are extracted within 200 km of the different stations listed in table B.3. The mean value of valid OCIO SCD (oclo_flag value set to 1 or 2, i.e. SZA between 85° and 92°) is then calculated for each day, in order to improve the signal to noise ratio. Coincidences with the ground-based data are obtained by selecting ground-based data that are within $\pm 1^\circ$ SZA of the mean daily satellite value.

Figure B.3 illustrates the SZA variability for GOME-2A pixels around two stations: Harestua (60°N) and Neumayer (71°S). The non-constant number of points with SZA > 85° (above the dotted line) throughout the year and the impact of the reduced swath configuration for GOME-2A in July 2013 can be seen. Several periods of the year (depending on the location) don't have any valid OCIO SCD pixels and these periods are longer after 2013.

Comparisons of the daily coincidences and of their monthly means are performed at each station for the whole time-series. Quantification through a linear regression analysis is performed both on daily and monthly points.

This approach of comparing the slant columns (instead of the vertical columns) relies on the assumption that satellite nadir and ground-based zenith sky light path are comparable at large SZA (Oetjen et al., 2011), i.e. that AMF_{sat_nadir} and AMF_{gb_zenith} are similar. Oetjen et al. calculated differences of ~4% for the two observation geometries between 89° and 91° SZA in NyAlesund.

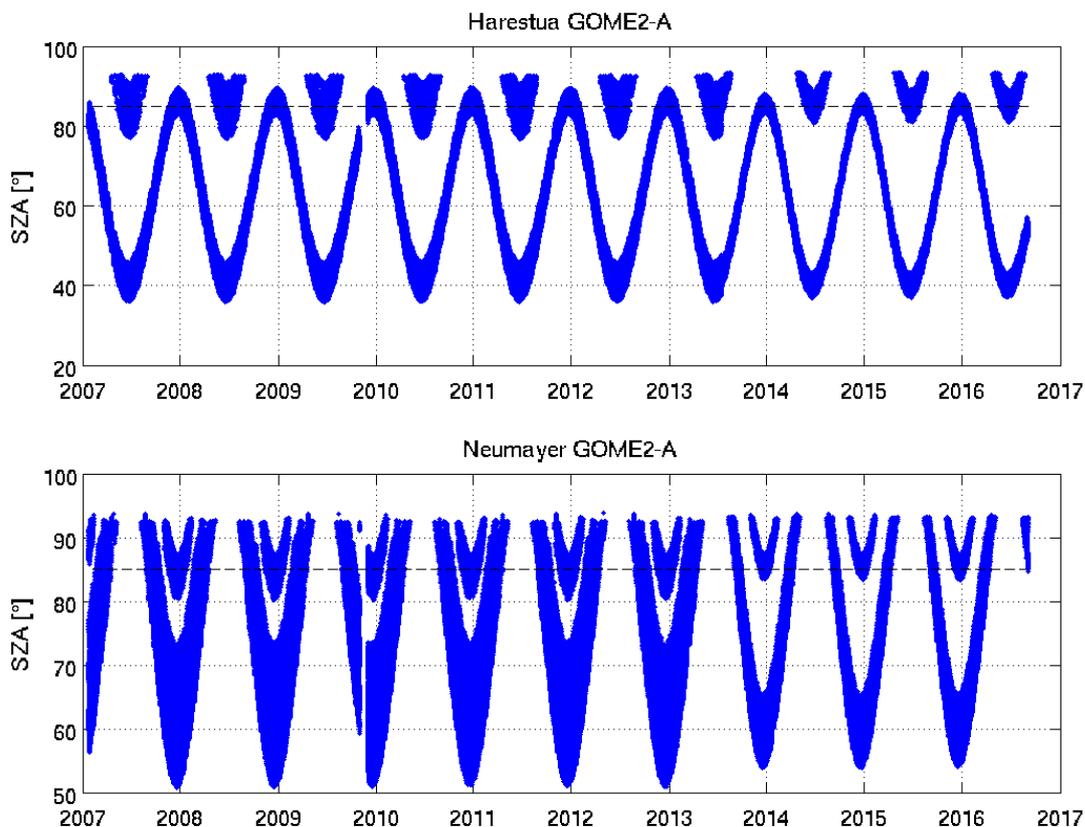


Figure B.3 Illustration of the SZA time evolution for all the pixels within a radius of 200 km around the station. In July 2013 GOME-2A swath is reduced to half of his nominal length, which impacts the coverage around the stations. The black dotted line corresponds to 85° SZA.

C. COMPARISON AGAINST GROUND-BASED ZENITH-SKY DOAS DATA

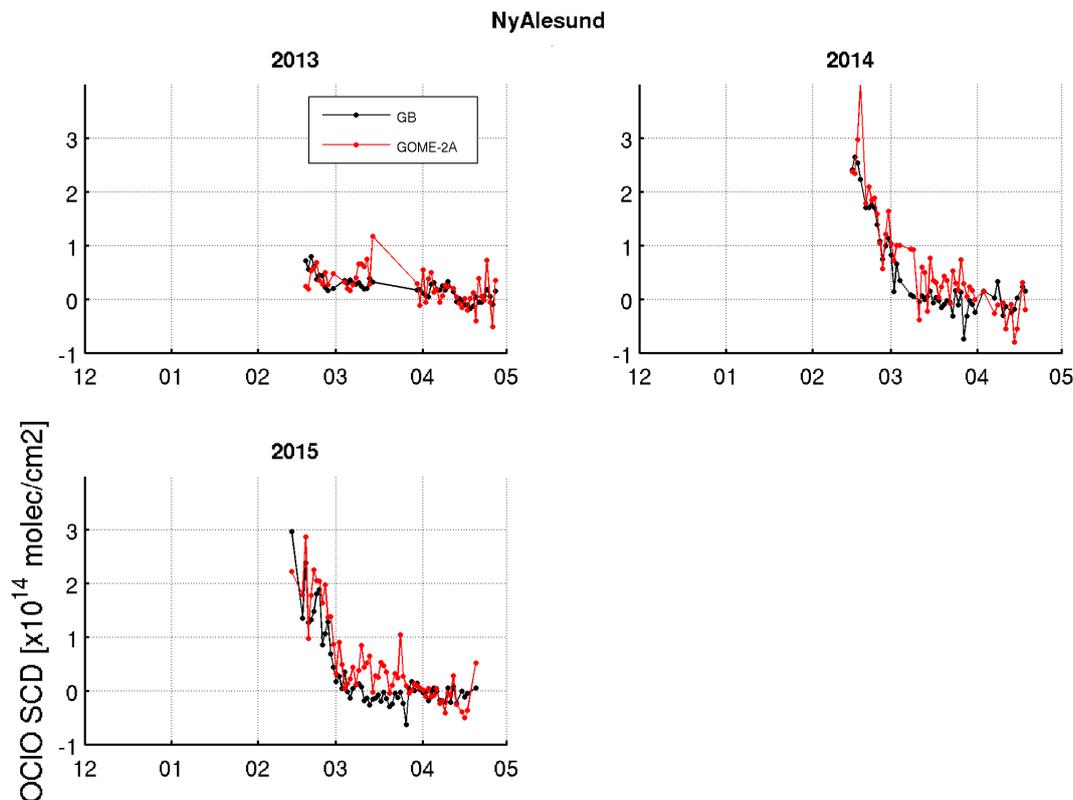
This chapter reports on comparisons of GDP 4.8 of GOME-2A/B OCIO slant column data against ground-based reference measurements acquired by zenith-sky looking UV-visible spectrometers.

C.1 OCIO columns around the Arctic

This section presents comparisons at three stations distributed around the Arctic Circle: Ny-Alesund on Spitsbergen, Kiruna in Sweden and Harestua in Norway. At all stations GOME-2A GDP 4.8, GOME-2B GDP 4.8 and the zenith-sky DOAS instruments capture similarly the seasonal cycle of OCIO, as well as monthly and day-to-day changes in OCIO SCD. Differences from year to year and station to station exist, but typical enhanced OCIO slant columns are found at the 3 sites in winter, with values up to 3×10^{14} molec/cm².

Ny-Alesund (78.9°N, 11.9°E)

IUP-Bremen operates a UV-VIS spectrometer in Ny-Alesund (Spitsbergen) since 1995. This instrument submit NO₂ and O₃ VCD as part of the NDACC network, and OCIO SCD have been analysed for 2013, 2014 and 2015, as presented in Richter et al. (2015) visiting scientist. The daily comparisons are presented in figure C.1.1, separated per year and for both GOME-2A (in red) and GOME-2B (in green). Both 2014 and 2015 show an enhanced OCIO signal in February (larger than 2×10^{14} molec/cm²) followed by a decrease, while 2013 does not show the chlorine activation.



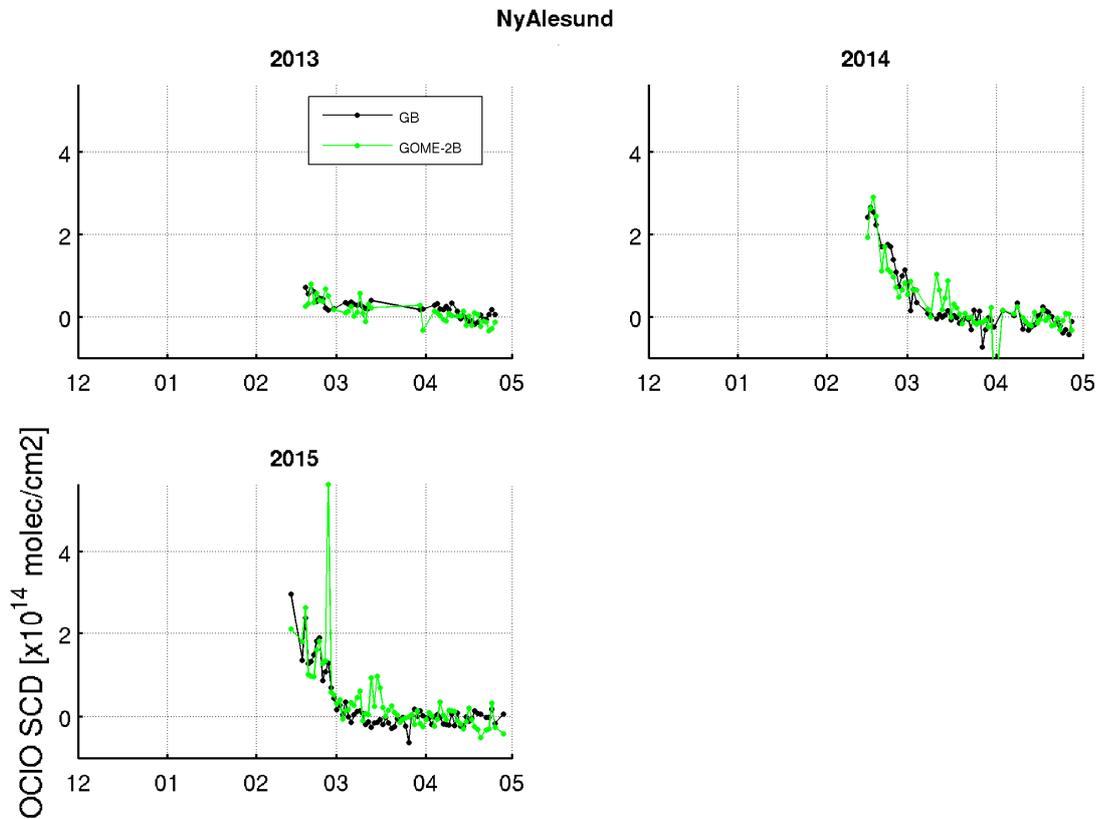


Figure C.1.1 Comparison of OCIO daily slant column measured at the NDACC NyAlesund station by GOME-2-A/B (GDP 4.8) and by the zenith-sky UVVIS spectrometer operated by IUPB. GOME-2A results in red; GOME-2B results in green. Different panels are given for every year.

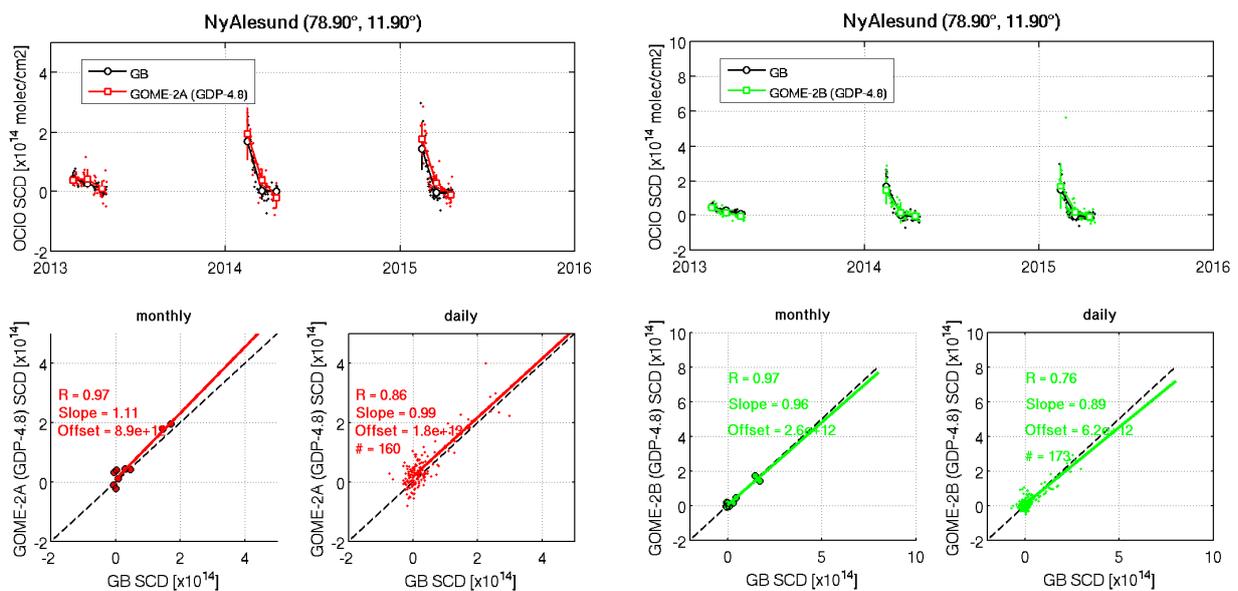


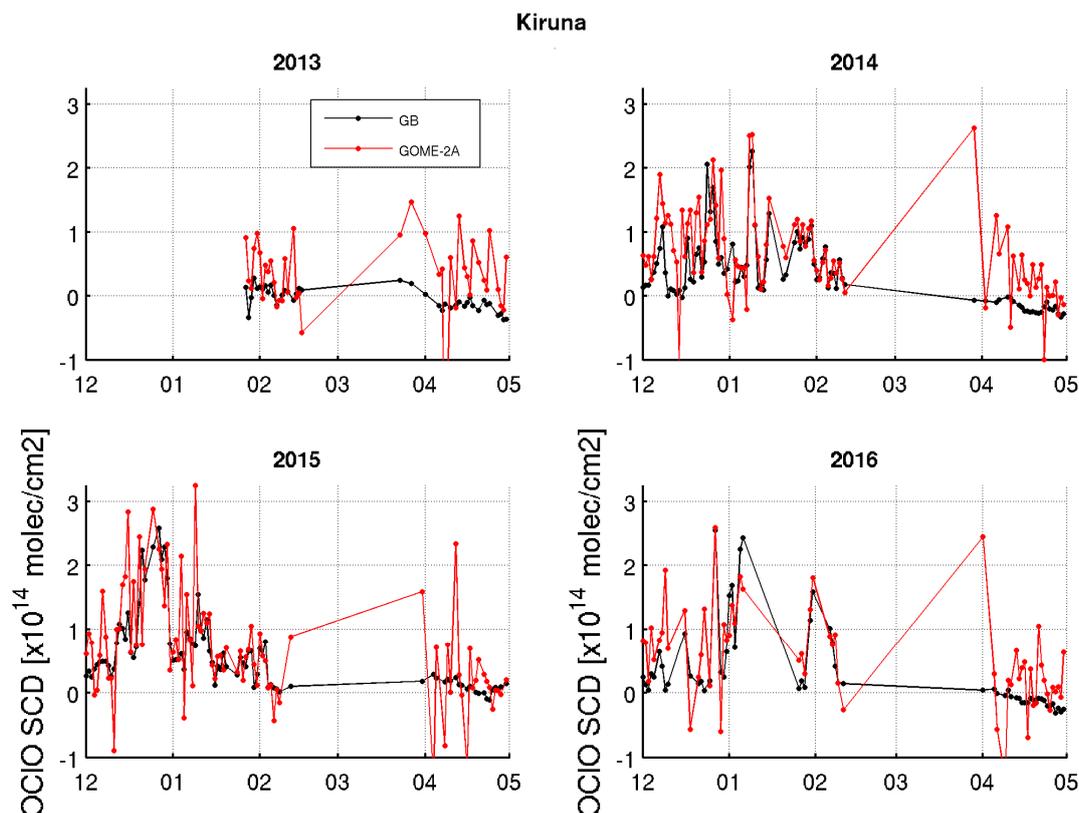
Figure C.1.2 Comparison of OCIO slant column measured at the NDACC NyAlesund station by GOME-2-A/B (GDP 4.8) and by the zenith-sky UVVIS spectrometer operated by IUPB. Left panel: GOME-2A results; right panel: GOME-2B results. In every panel, top graph: OCIO column time series; bottom graphs: monthly mean and daily mean scatter plots between GOME-2 and ground-based data.

Figure C.1.2 shows the whole time-series and the corresponding scatter plots, for both the daily and monthly mean comparisons. Statistics analysis leads to correlation coefficients from 0.76 to 0.86 for GOME-2B and GOME2-A daily comparisons and slopes for linear regression from 0.89 to 0.99. When doing monthly mean comparisons, correlation coefficients reach 0.97 and slopes 0.96 and 1.11.

Kiruna (67.9°N, 20.4°E)

MPIC operates a UV-VIS spectrometer in Kiruna (Sweden) since 1996. OCIO SCD have been analysed for 2013, 2014, 2015 and 2016 (between 2009 and 2013 the instrument was not operated on many days due to detector problems). The daily comparisons are presented in figure C.1.3, separated per year and for both GOME-2A (in red) and GOME-2B (in green). As for Ny-Alesund, both 2014, 2015 and 2016 show an enhanced OCIO signal (with peaks larger than $2\text{-}3 \times 10^{14}$ molec/cm²) while 2013 does not seem to show the chlorine activation. GOME-2A is more noisy than GOME-2B, especially outside the chlorine activation period (e.g. 2013 and points in April of the other years), but both sensors follow nicely the enhanced OCIO signals in December 2013/early 2014, December 2014/early 2015 and December 2015/early 2016. The gap in the comparisons around February, March and part of April is related to the GOME-2 pixels SZA being smaller than 85° in that period, and thus not selected by the OCIO validity flag (see table B.2). Difference for GOME-2A and GOME-2B are related to the smaller GOME-2A swath after July 2013 and the 50 minutes difference of the 2 instruments orbits. Moreover, GOME-2A degradation could also play a role in more noisier OCIO columns.

Figure C.1.4 shows statistics analysis that leads to correlation coefficients from 0.62 to 0.77 for GOME-2A and B daily comparisons and slopes from 0.83 to 0.86. For the monthly mean comparisons, correlation coefficients reach 0.90 and 0.93 and slopes 0.80 and 0.86.



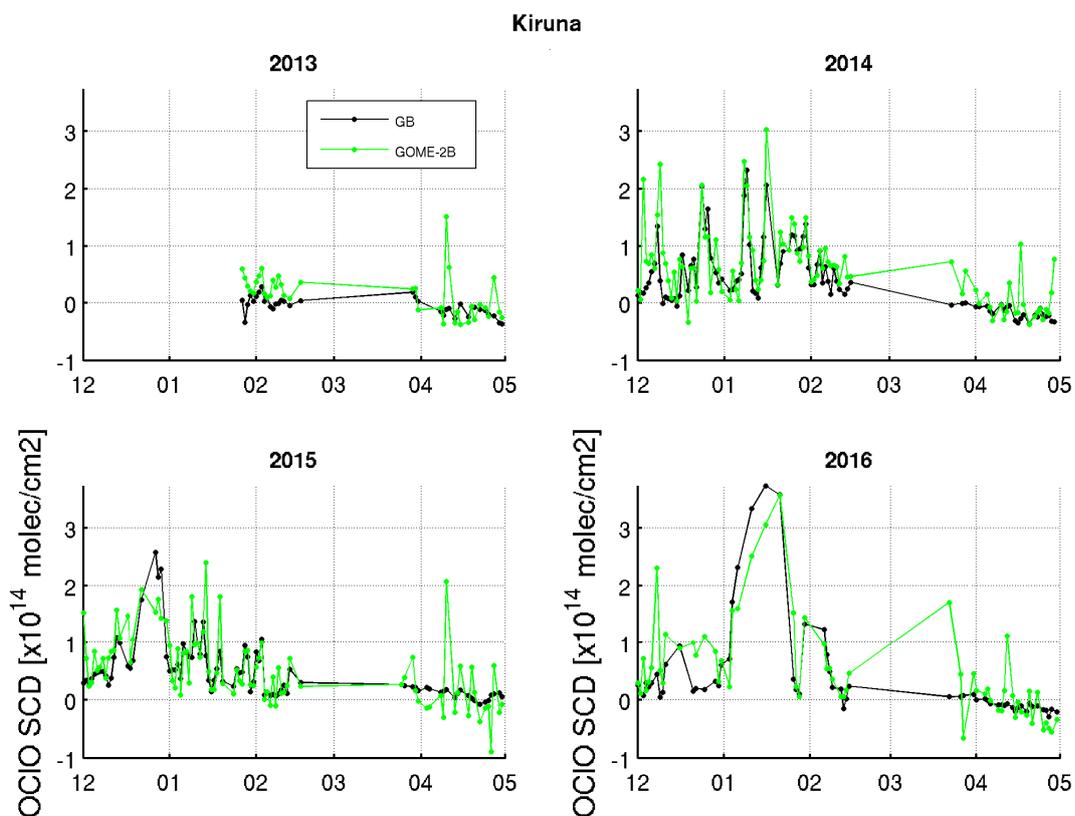


Figure C.1.3 As figure C.1.1 but for the ground-based data of the Kiruna MPIC instrument.

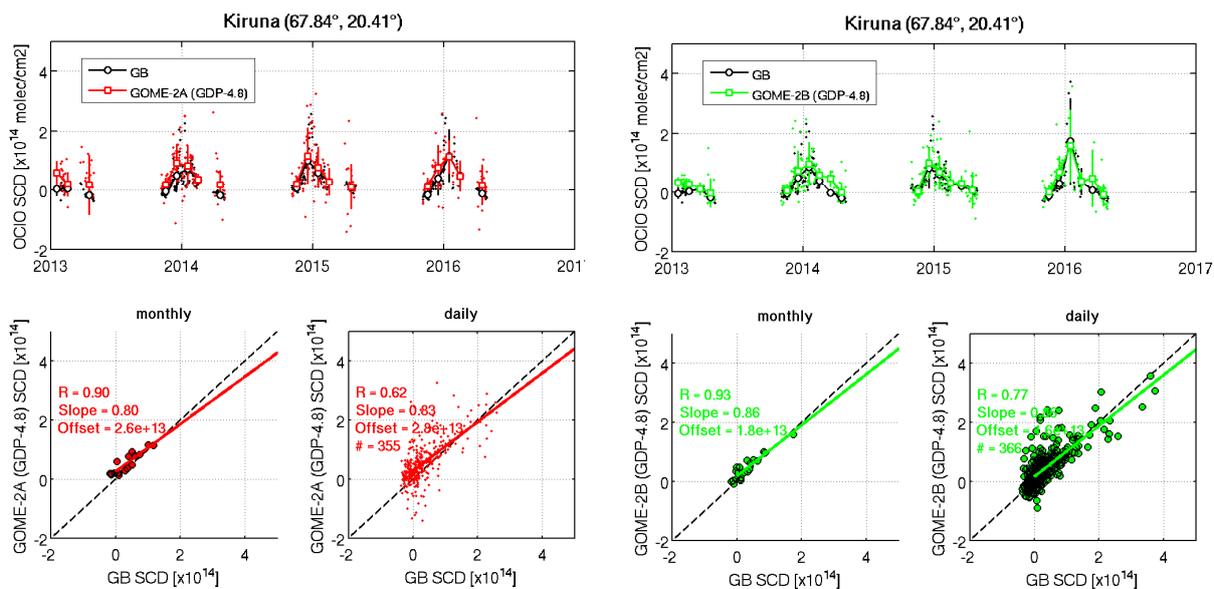
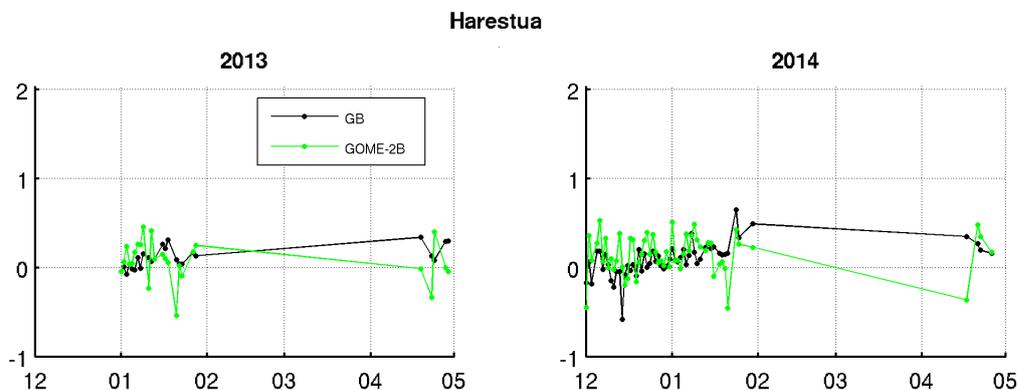
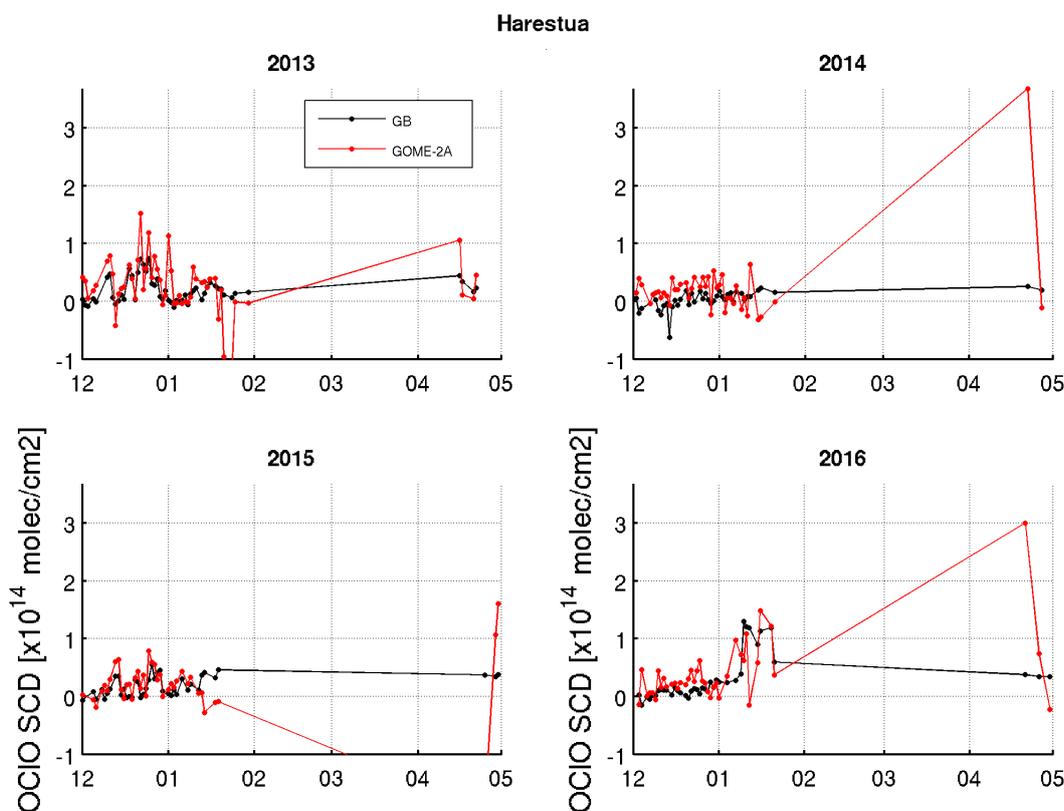


Figure C.1.4 As figure C.1.2 but with the ground-based data of the Kiruna MPIC instrument.

Harestua (60.22°N, 10.75°E)

BIRA-IASB operates a UV-VIS spectrometer in Harestua (Norway) since the '90 and submits NO₂ and O₃ VCD as part of the NDACC network. End of 2012 a new instrument has been installed with an improved signal to noise ratio, and OCIO SCD have been analysed since then. The daily comparisons are presented in figure C.1.5 and the statistical analysis is presented in figure C.1.6. Unlike Ny-Alesund and Kiruna, the chlorine activation in 2014 and 2015 can not be seen in Harestua, probably due to the polar vortex not extending as low as 60°N. In 2016 on the other hand, a clear enhancement is visible from the ground and from GOME-2A and B in January (with a peak ~1.3-1.5 x10¹⁴ molec/cm²). Unfortunately the gap in the GOME-2 data from February to May (related to the GOME-2 pixels SZA being smaller than 85°, see figure B.3) prevents us to see the other OCIO SCD peaks, seen by the ground-based instrument. The statistics analysis indicates correlation of 0.70 for GOME-2B daily comparisons with a slope of 0.81, similar to results at the other stations.



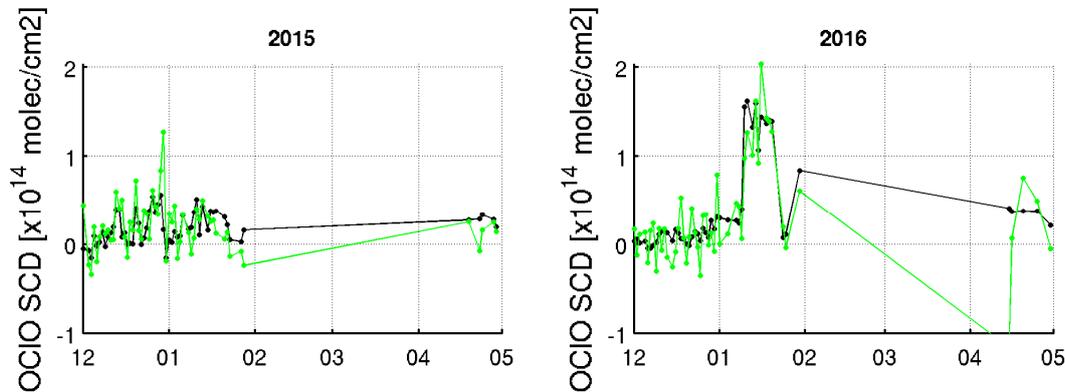


Figure C.1.5 As figure C.1.1 but for the ground-based data of the Harestua BIRA-IASB instrument.

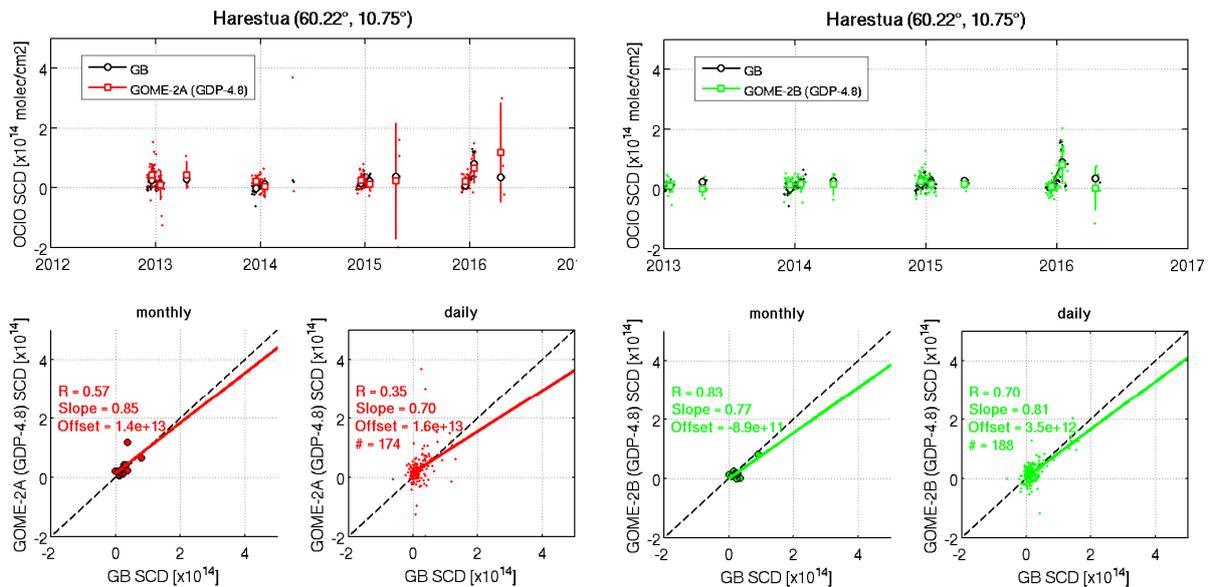


Figure C.1.6 As figure C.1.2 but with the ground-based data of the Harestua BIRA-IASB instrument.

C.2 OCIO column in Antarctica

Data of five stations have been collected for the validation of the GOME-2 columns around Antarctica. In this region the OCIO signal is stronger in the winter months, with values up to $5-10 \times 10^{14}$ molec/cm², when the stations are within the polar vortex. The vortex, which is one of the most important prerequisites for the chemical destruction of stratospheric ozone above this region, is created by the large-scale descent of cold air masses during winter, with the Coriolis force leading to strong circumpolar winds that prevent inner vortex air from mixing with outer vortex air. While the inhomogeneous distribution of landmasses in the Northern Hemisphere leads to frequent disturbances of the Arctic vortex by vertical propagation of planetary waves, the Antarctic vortex usually remains stable and more or less symmetric until at least late November.

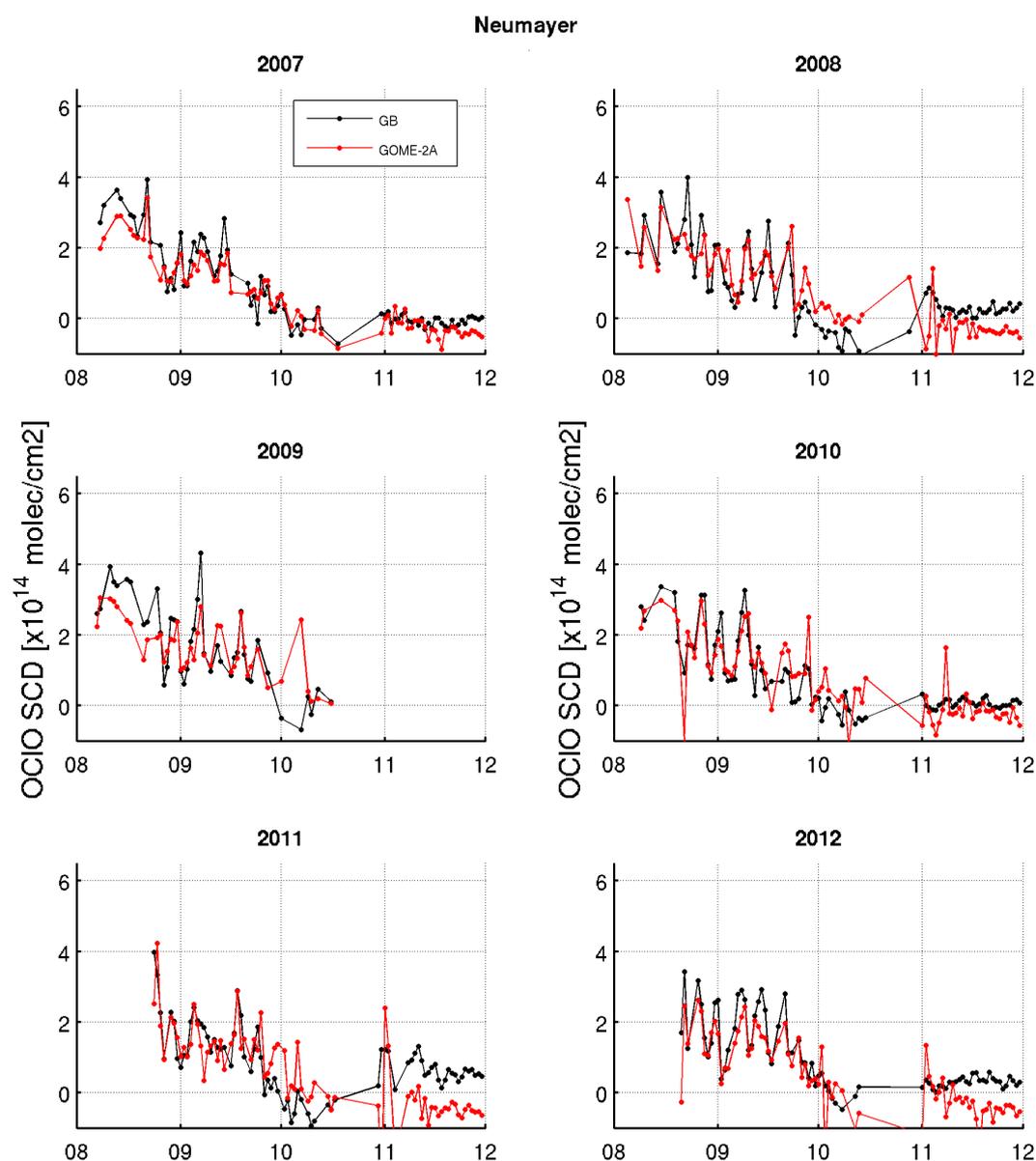
Neumayer (70.62°S, 8.27°W)

IUP-Heidelberg operates a UV-VIS spectrometer in German research station Neumayer (the ice shelf in the Atlantic sector of the Antarctic continent) since the '90 (Friess et al., 2005). OCIO SCD have been analysed for the whole GOME-2 time-series (2007-2016) showing enhanced OCIO signals between August and October, when the polar vortex is over the station. The daily comparisons for August to December are

presented in figure C.2.1, separated per year and for both GOME-2A (in red) and GOME-2B (in green). Every year show an enhanced OCIO signal (from ~ 2 and up to 4 and 6×10^{14} molec/cm²) in August and September, followed by a decrease, and the daily variations are sampled in a very coherent way from the ground and from space. A gap in the GOME-2A data in October is present since 2013, due to reduced swath, and no overpass pixels within 300 km are present for both sensors between May and end of July, with the result of missing the start of the chlorine activation.

The day to day variability seen in the ground-based data is well reproduced by both GOME-2 sensors, especially during the activated period. Larger differences in the first comparison days in August are found in 2014 and 2016 for both GOME-2, and in 2013 for GOME-2A, with smaller satellite columns. Generally smaller (and negative) OCIO SCDs are retrieved by the satellites during November, outside of the chlorine activation period. Ground-based data at the end of the time-serie (since November 2015) seems un-usually high in Neumayer and the results of those months should be interpreted with care.

Figure C.2.2 shows the statistics analysis that leads to correlation coefficients from 0.69 to 0.80 for GOME-2A and B daily comparisons and slopes around 0.67-0.63. For the monthly mean comparisons, correlation coefficients reach 0.84 and 0.91 and the slopes stays around 0.69 and 0.68.



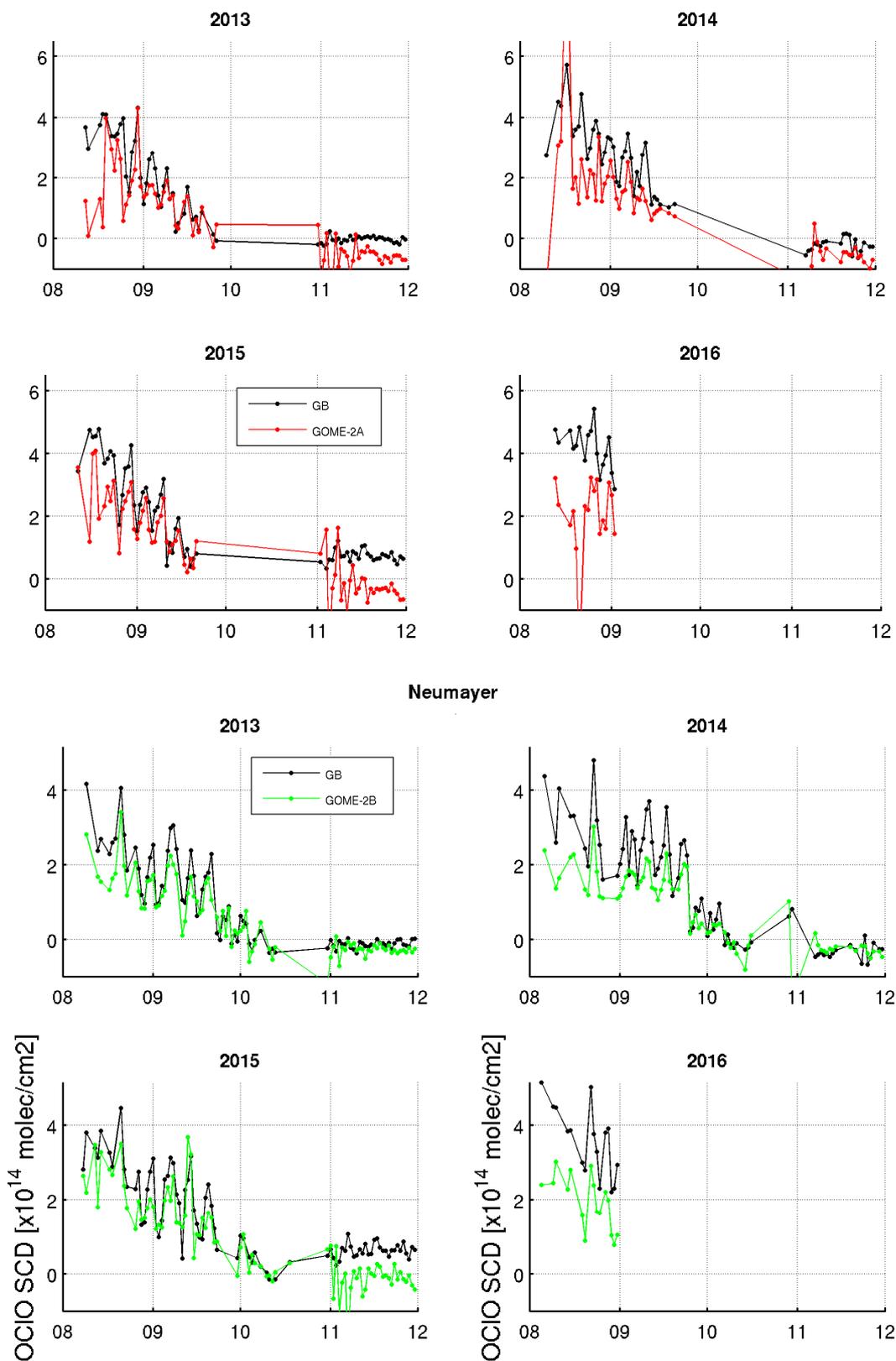


Figure C.2.1 Comparison of OCIO daily slant column measured at the NDACC Neumayer station by GOME-2-A/B (GDP 4.8) and by the UVVIS spectrometer operated by IUPH. GOME-2A results in red; GOME-2B results in green. Different panels are given for every year.

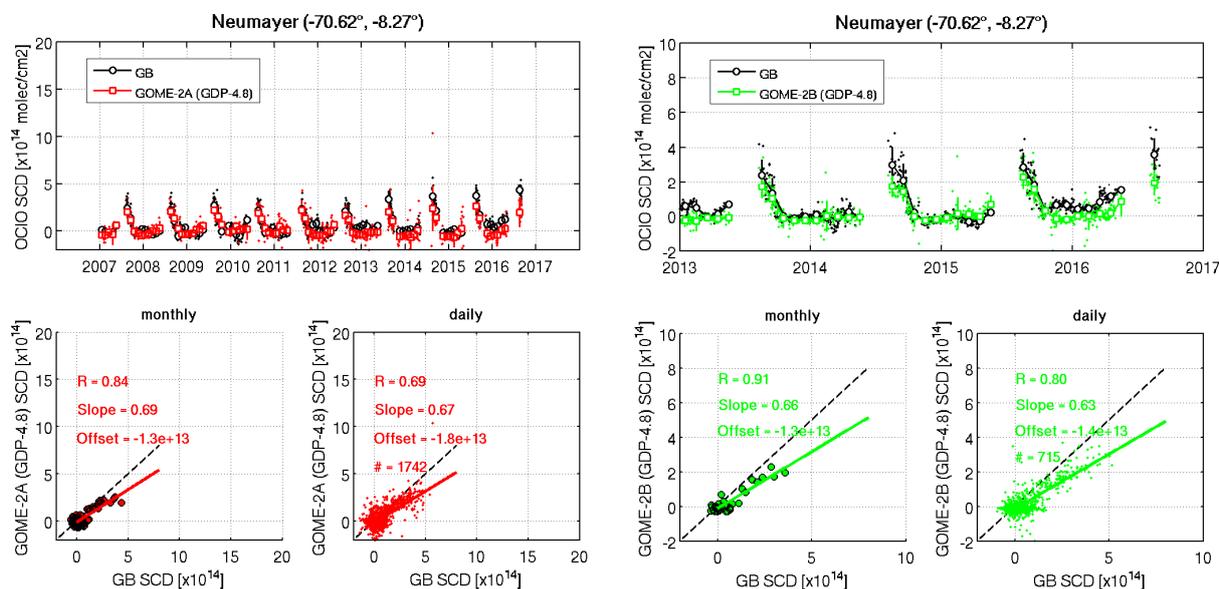


Figure C.2.2 Comparison of OCIO total column measured at the NDACC Neumayer station by GOME-2-A/B (GDP 4.8) and by the UVVIS spectrometer operated by IUPH. Left panel: GOME-2A results; right panel: GOME-2B results. In every panel, top graph: OCIO column time series; bottom graphs: monthly mean and daily mean scatter plots between GOME-2 and ground-based data.

Arrival Heights (77.83°S, 166.65°W)

IUP-Heidelberg operates a UV-VIS spectrometer in Arrival Heights (78°S, 167°E), part of the New Zealand station Scott Base on Ross Island since the '90 (Friess et al., 2005). Another instrument is present at the station, operated by NIWA (Kreher et al., 1996). OCIO SCD have been analysed for the whole time-series (2007-2016 with a few gaps) for both instruments, and they detect an enhanced OCIO signal between August and October. However, it should be reminded that while the IUPH instrument retrieves OCIO in the UV (between 364-391nm), the NIWA instrument only covers the visible range, and measures OCIO in the 402-440nm range (Kreher et al., 1996, Friess et al., 2005). The statistical error in OCIO SCDs during twilight is of the order of 2×10^{13} molec/cm² (Friess et al., 2005). As we focus on SCD, differences in the retrieved OCIO should be expected due to the different wavelength regions, and we treat hereafter the 2 datasets separately. It should be noted that the IUPH data are given every 20 minutes during the day and every 2-5 minutes during twilight, while the NIWA data are reported every 5° SZA. The comparison method described in Section B.2 has thus been adapted for the NIWA comparison and ground-based pairs are searched for SZA within 5° of the daily mean satellite SZA value.

Figure C.2.3 shows the time-series of the two ground-based datasets, in order to have a feeling of the differences. The first line presents the whole time-series, from 2006 to end of October 2016. Both datasets show large enhancement of the OCIO SCD in the August to October period, with the NIWA dataset seeing larger columns until August 2012. In the period 2012-2014, the two data-sets are more coherent than before. As can be better seen in the second and third line with zooms over 2 years periods, some instrumental instabilities are present in early 2011 and in late 2011/early 2012 in the IUPH dataset (grey points with SZA smaller than 85°).

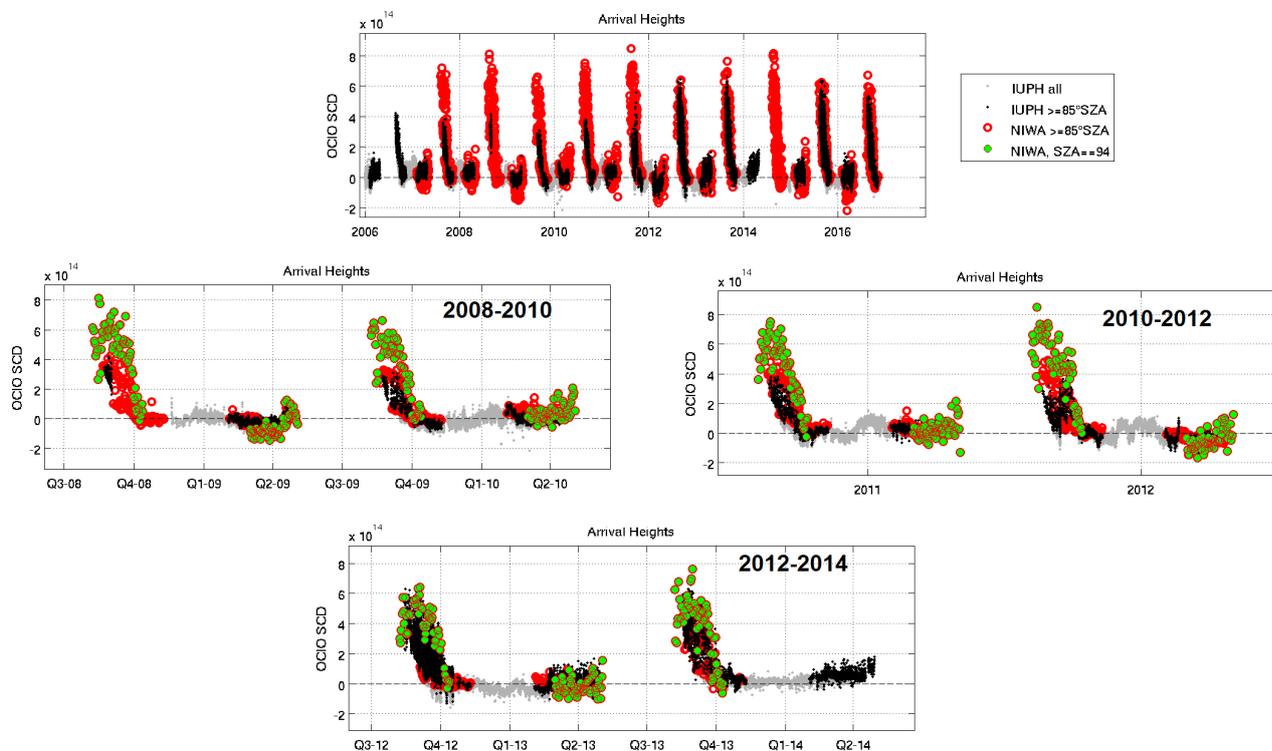
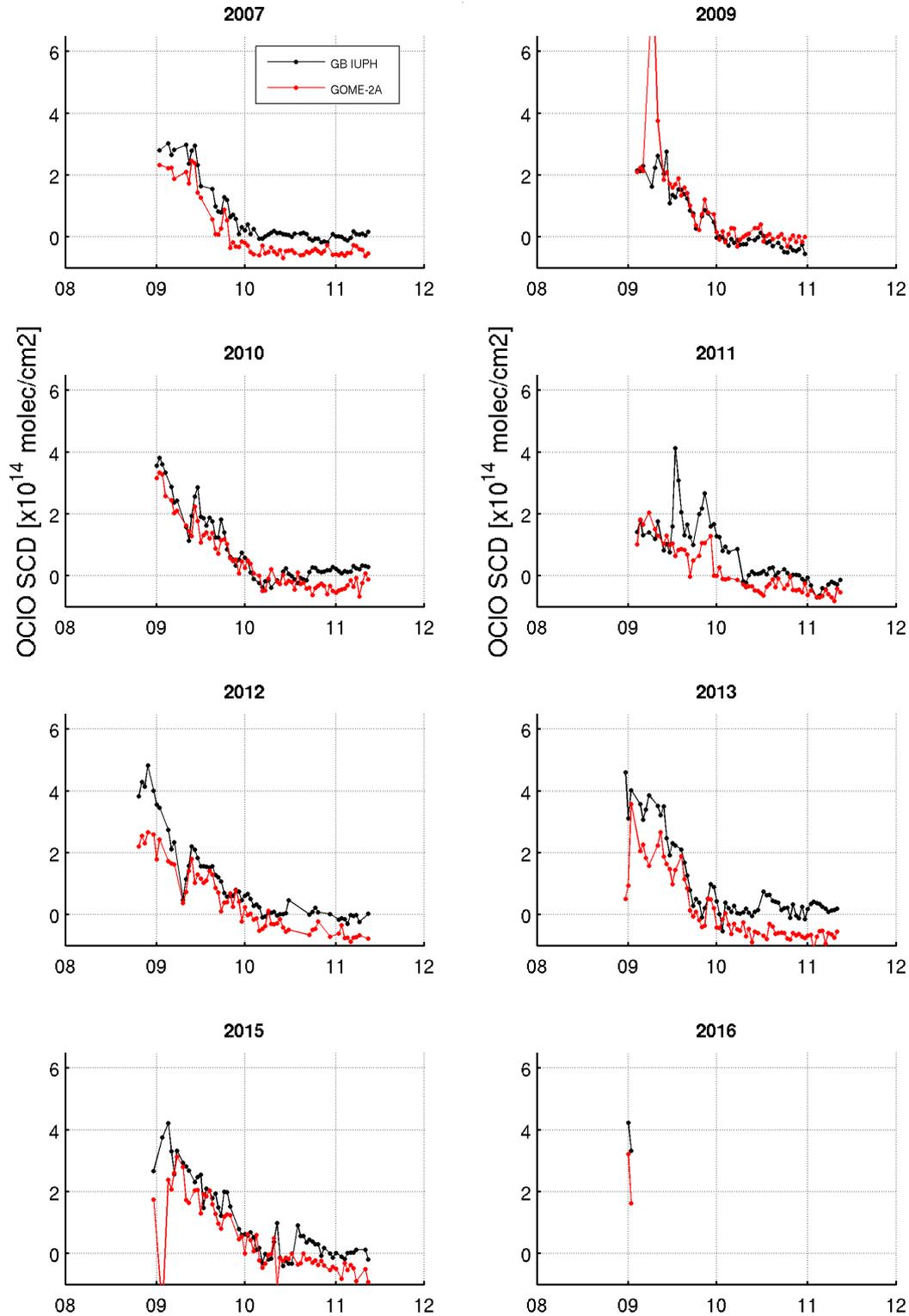


Figure C.2.3 Time-series of the 2 ground-based data at the Arrival Heights station.

The daily comparisons for August to December are presented in figure C.2.4 for the IUPH instrument and in C.2.5 for the NIWA instrument. For both figures, every year show an enhanced OCIO signal (from ~ 2 and up to 4 and 6×10^{14} molec/cm²) in August and September, followed by a decrease, and the daily variations are sampled in a very coherent way from the ground and from space. A gap in the GOME-2A data in October is present since 2013, due to reduced swath. As discussed above, the IUPH data in 2011 and beginning of 2012 should be considered with care.

ArrivalHeights IUPH



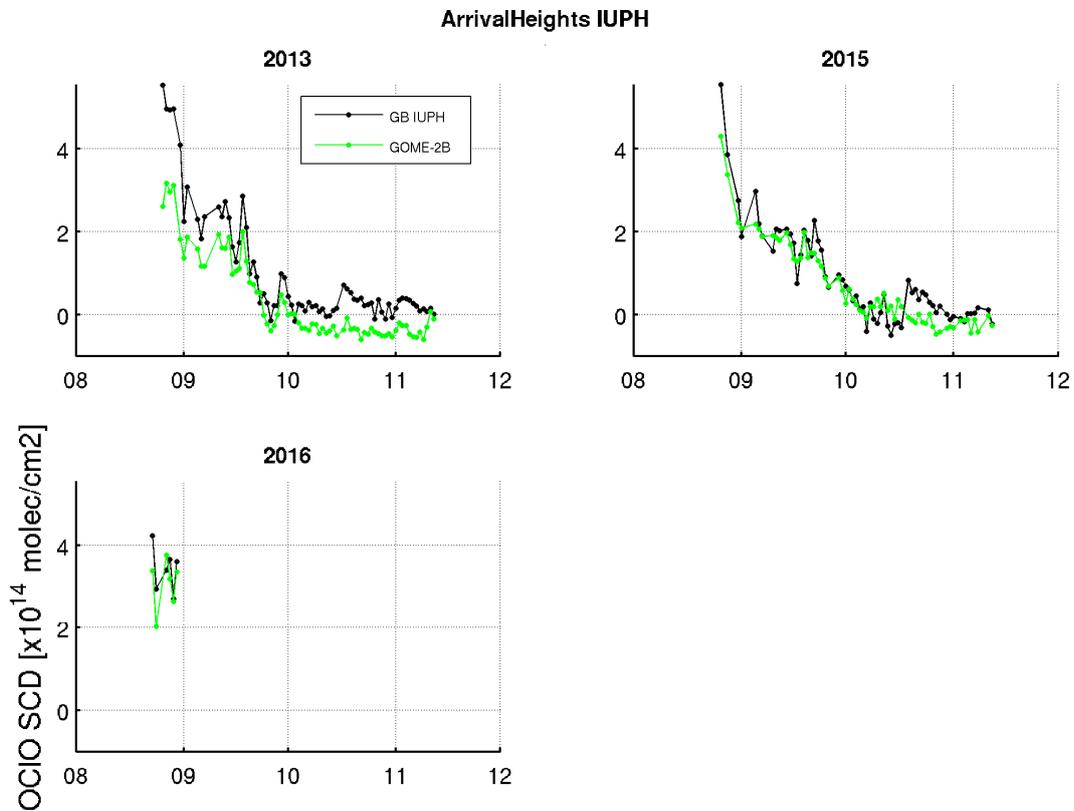
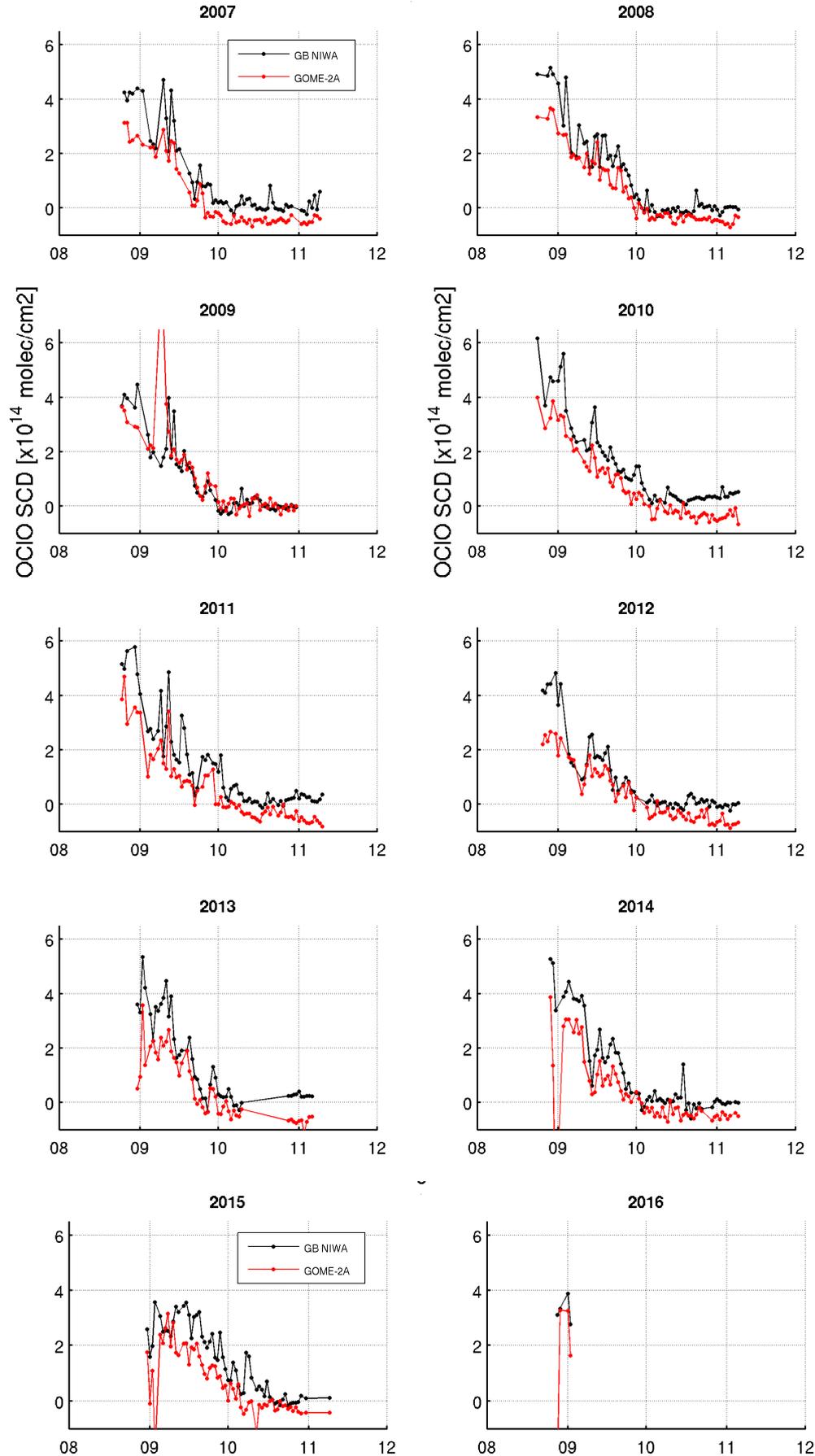


Figure C.2.4 As figure C.2.1 but for the ground-based data of the Arrival Heights IUPH instrument.

ArrivalHeights NIWA



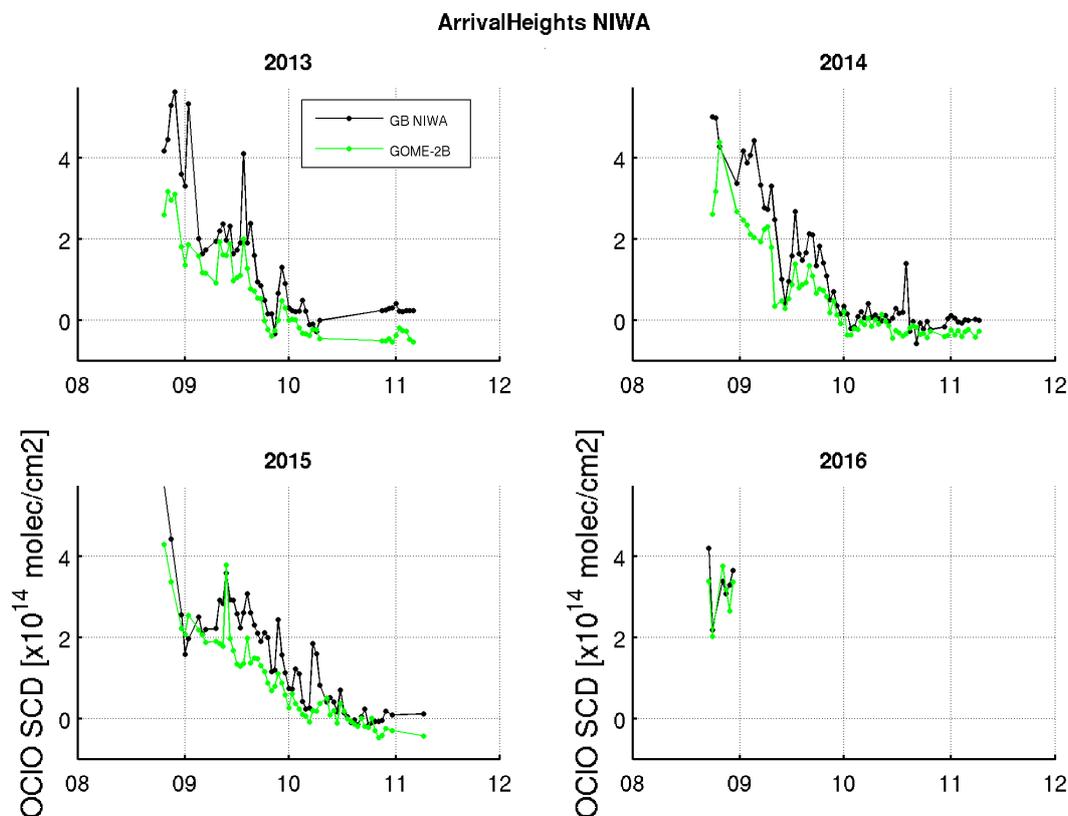


Figure C.2.5 As figure C.2.1 but for the ground-based data of the Arrival Heights NIWA instrument.

Figures C.2.6 and C.2.7 show the statistics analysis that leads to correlation coefficients from 0.82 to 0.85 for GOME-2A and B daily comparisons and linear regression slopes around 0.67-0.65 for the comparisons with the IUPH data. For the monthly mean comparisons, correlation coefficients reach 0.90 and 0.96 and the slopes are around 0.66 and 0.73.

The comparison with NIWA data shows correlation coefficients from 0.82 to 0.85 for GOME-2A and B daily comparisons and linear regression slopes around 0.79-0.73, while the monthly mean comparisons show correlations of 0.9 and 0.96 and slopes of 0.71 and 0.75. The results of the two datasets are thus very coherent.

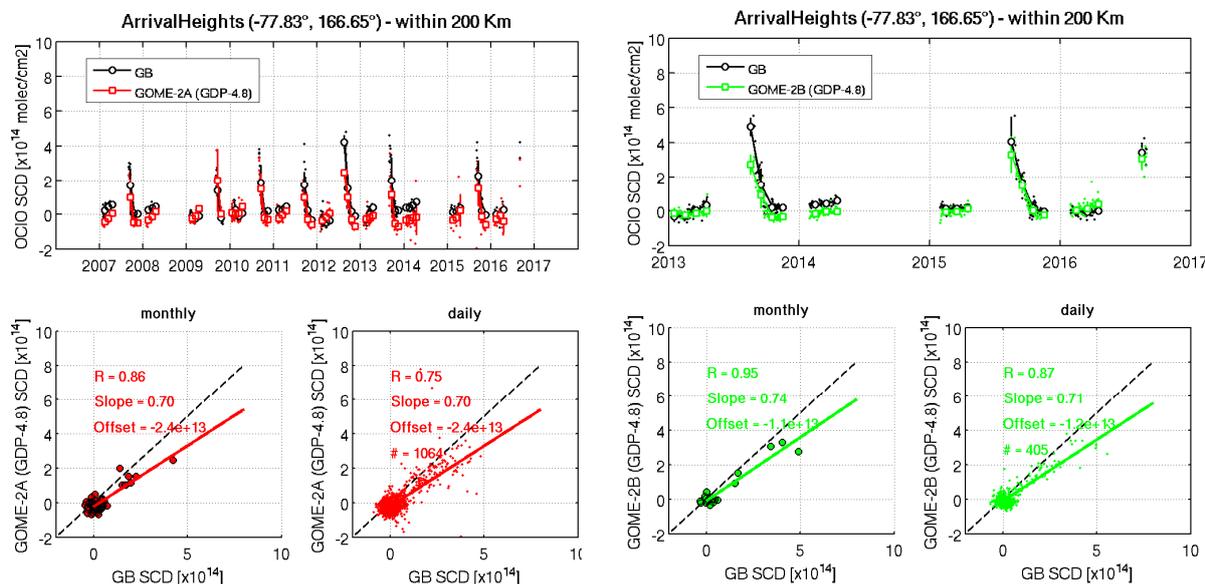


Figure C.2.6 As figure C.2.2 but with the ground-based data of the Arrival Heights IPUH instrument.

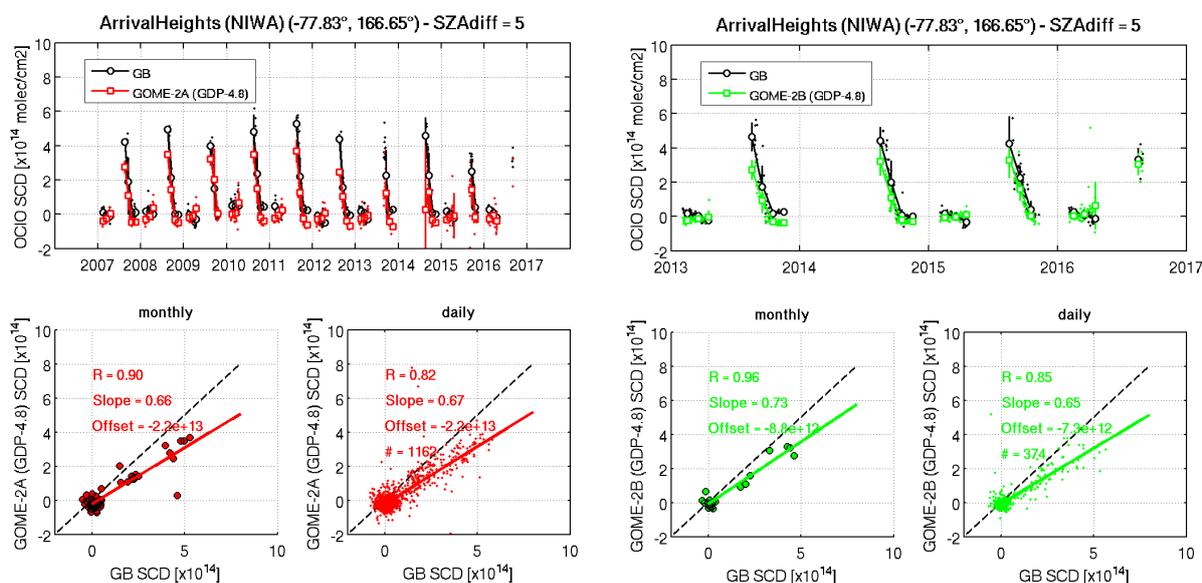


Figure C.2.7 As figure C.2.2 but with the ground-based data of the Arrival Heights NIWA instrument.

Belgrano (77.9°S, 34.6 °W)

INTA operates a UV-VIS spectrometer in Belgrano II station, the Argentinian station situated on the coast of the Antarctic continent in the Weddell Sea area. Belgrano is representative of an in-polar vortex station during winter-spring season until the vortex breakdown (Yela et al., 2005, Punterura et al. 2014). The UV instrument is measuring since February 2011 and OClO SCD have been analysed by INTA for 2011 and 2015. Ground-based SCD are made between January and May and from mid August to end of the year, outside of the polar night period (mid April to end of August). The first period is an OClO free period, while the second is capturing the decrease (from $\sim 6 \times 10^{14}$ molec/cm²) of the chlorine activation in August and September. The latter is seen in a very coherent way both from ground and from space with the 2 GOME-2

instruments, as seen in the daily comparisons of figure C.2.8. Larger differences between GOME-2A and the ground-based OCIO SCD are seen in 2011 (between 0.5 to 1×10^{14} molec/cm²) but it should be mentioned that in 2011 also the ground-based OCIO signal in the first period is unexpectedly larger (see C.2.9), and should thus be interpreted with care.

Figure C.2.9 shows the statistics analysis that leads to correlation coefficients from 0.82 to 0.89 for GOME-2A and B daily comparisons and slopes around 0.79-0.80. For the monthly mean comparisons, correlation coefficients reach 0.95 and 0.99 and the slopes stays around 0.93 and 1.

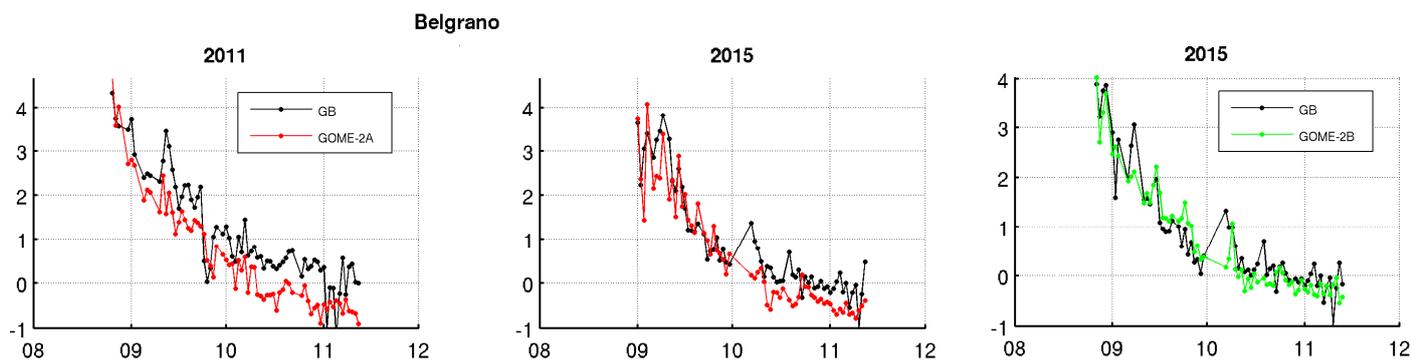


Figure C.2.8 As figure C.2.1 but for the ground-based data of the Belgrano INTA instrument.

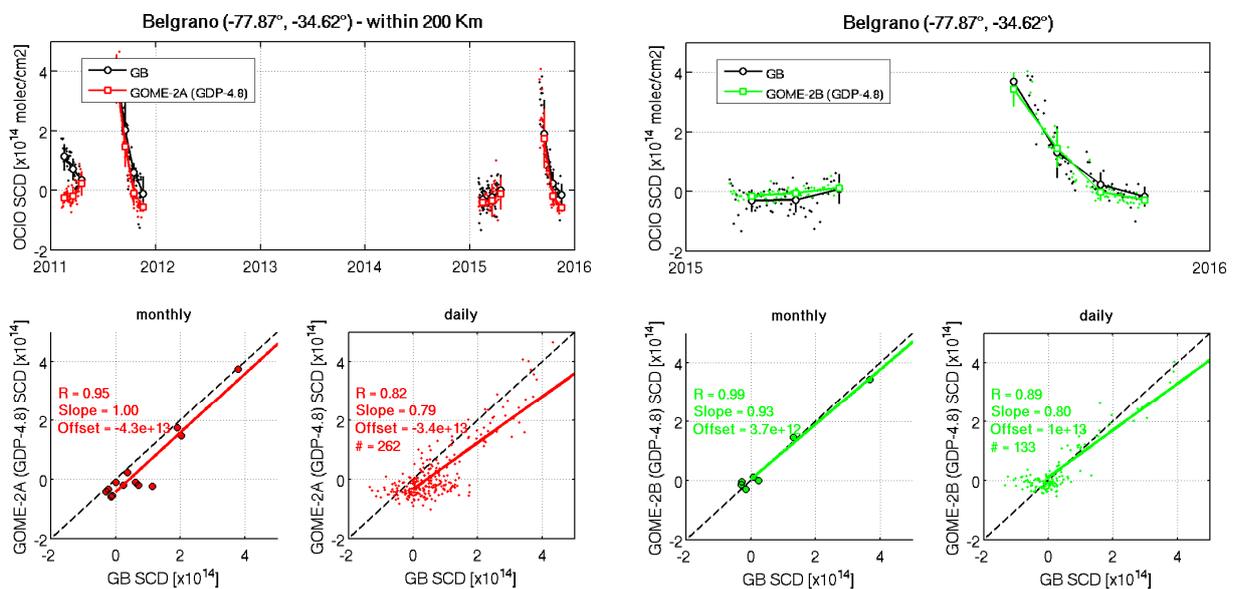


Figure C.2.9 As figure C.2.1 but with the ground-based data of the Belgrano INTA instrument.

Marambio (64.3°S, 56.7°W)

INTA operates a UV-VIS spectrometer at the Argentinian Marambio station, in Marambio Island (Graham Land, Antarctic Peninsula) since 2015. Marambio is frequently located in the vortex edge region and alternates vortex air masses with mid-latitude air masses. The OCIO has been processed for 2015 and shows an enhanced signal in June, August and September, with a gap in the data in July. When selecting only the ground-based and satellite points as discussed in Section B.2, the daily comparisons (figure C.2.10 (a) and (b)) show a clear OCIO enhancement in August and September. Day to day variability of several 1×10^{14} molec/cm² can be seen in panel (b) during the activated period, and the sawtooth behavior could indicate

sampling of air masses that are on the edge of the Antarctic polar vortex. The ground-based data seems more sensitive to these rapid changes, with generally higher peaks than both GOME-2A and GOME-2B. The averaging of the satellite data within 200 km could mix air inside and outside the vortex, and thus a test with a selection of GOME-2 pixels within 50 km of Marambio station is done and presented in panel (c) in order to try to reduce difference in vortex conditions.

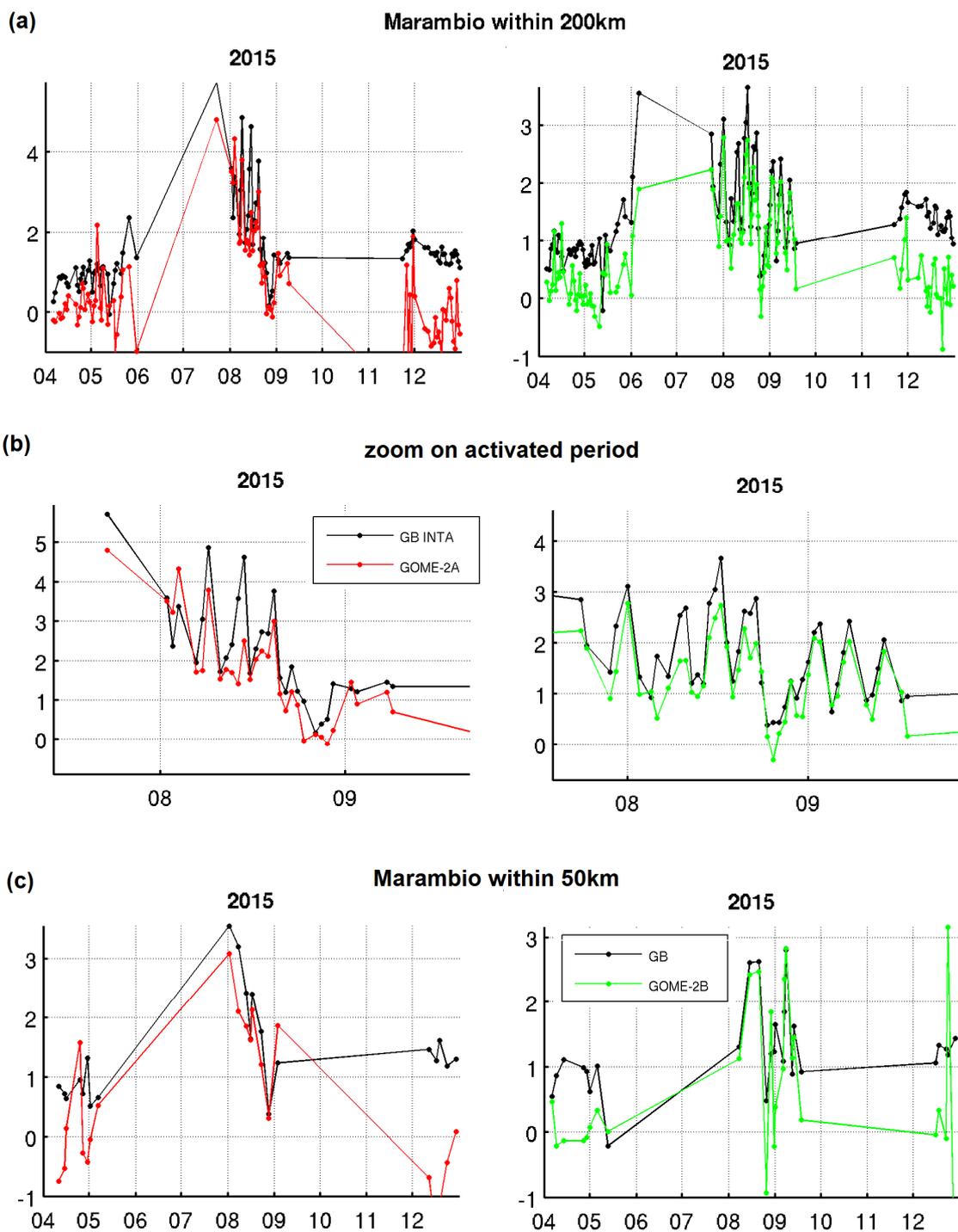


Figure C.2.10 Comparison of OCIO daily slant column measured at the Marambio station by GOME-2-A/B (GDP 4.8) and by the zenith-sky UVVIS spectrometer operated by INTA. Left panel: GOME-2A results in red; right panel: GOME-2B results in green. The different lines correspond to: (a) the whole dataset for a selection of GOME-2 pixels within 200 km

around the station; (b) a zoom over the chlorine activated period and (c) as line (a) but for a selection of pixels within 50 km.

The results of the statistics analysis in both 200 km and 50 km cases are presented in figures C.2.11 and C.2.12. In the first case the correlation coefficients ranges from 0.70 to 0.72 for GOME-2A and B daily comparisons with slopes around 0.85-0.94. For the second case, the number of daily points are reduced from ~100 to ~20, with a reduced correlation coefficient (around 0.54/0.65) but the slopes are closer to one (0.98 and 1.09). For the monthly mean comparisons, the number of points is small and the values have to be considered with care.

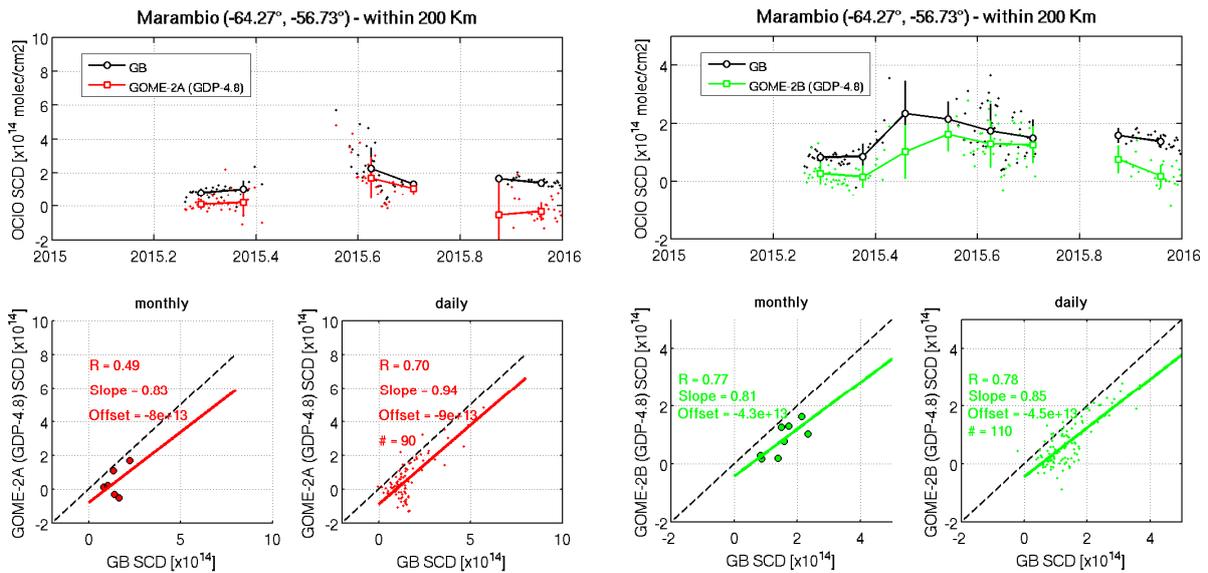


Figure C.2.11 Comparison of OCIO total column measured at the Marambio station by GOME-2-A/B (GDP 4.8) within 200 km and by the zenith-sky UVVIS spectrometer operated by INTA. Left panel: GOME-2A results; right panel: GOME-2B results. In every panel, top graph: OCIO column time series; bottom graphs: monthly mean and daily mean scatter plots between GOME-2 and ground-based data.

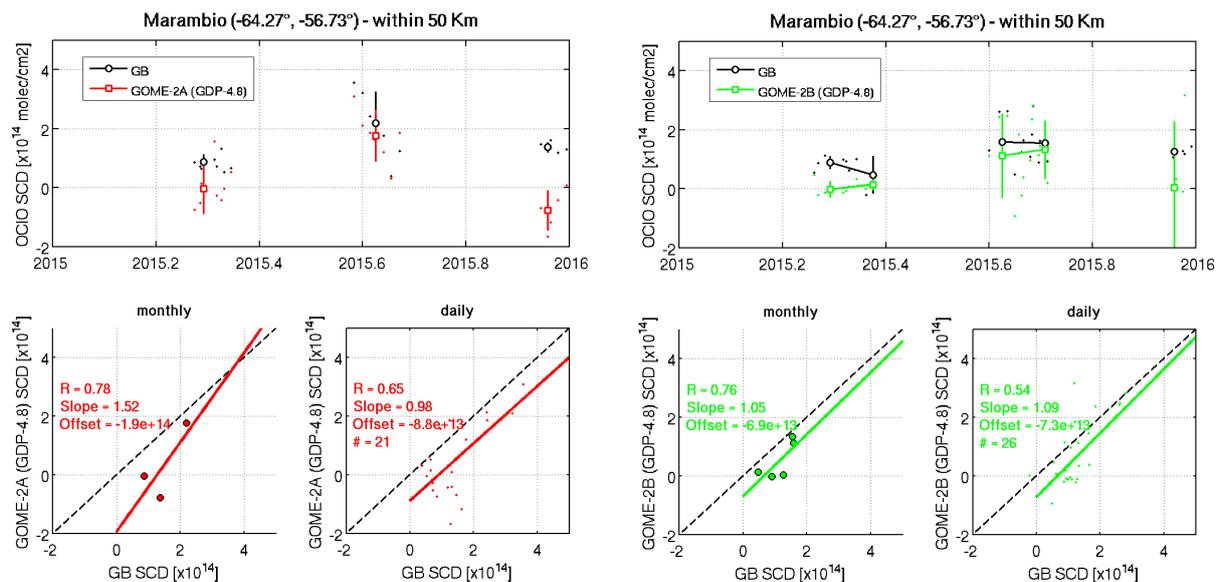


Figure C.2.12 As figure C.2.11 but reducing the selection criteria of the GOME-2 data around the Marambio station to 50 km instead of 200 km.

C.3 Comparisons summary

The individual comparisons described in the previous sub-sections for Arctic and Antarctic stations, can be synthesized in order to have a “global” view of the quality of the GOME-2 GDP 4.8 OCIO SCD product. Figures C.3.1 and C.3.2 show the correlations and the slopes of daily and monthly linear regressions of the GOME-2A and GOME-2B versus ground-based zenith-sky SCD data, as a function of the latitude of the stations (from left to right the latitude value is increasing). Daily comparisons are shown in black, while monthly mean comparisons are shown in red. These figures show very coherent agreement of GOME-2A and GOME-2B results with slopes around or better than 0.7, i.e. underestimation of less than 30% compared to the ground-based data, which is within the target accuracy of 50% and within/close to the optimal accuracy of 30%. This underestimation seems larger in the Southern Hemisphere, with the exception of Marambio, which is a challenging station affected by different situations of the polar vortex, and South Atlantic Anomaly affecting the satellite data. In the Northern Hemisphere the results are more variable and dependent on the station.

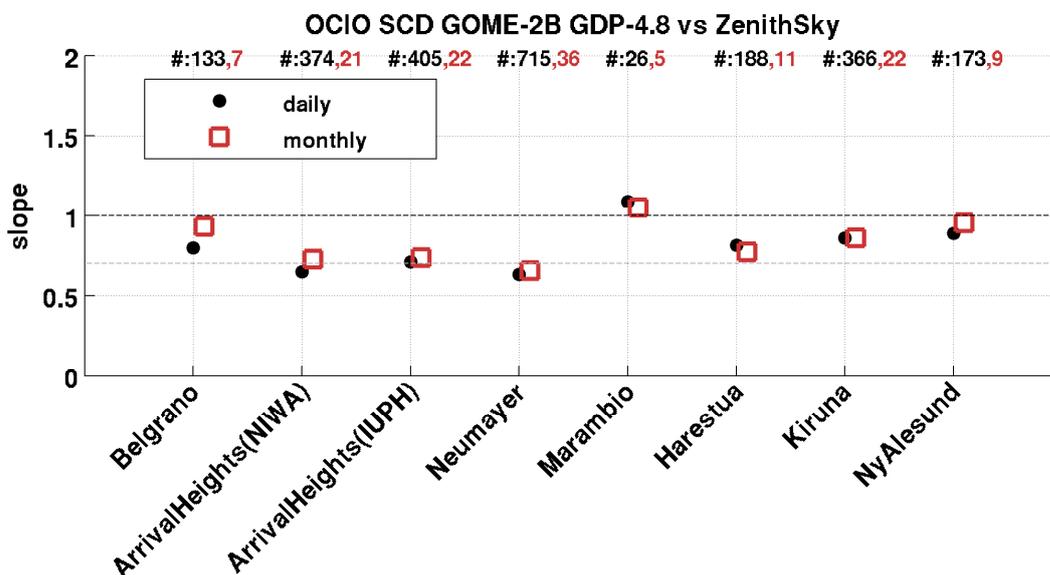
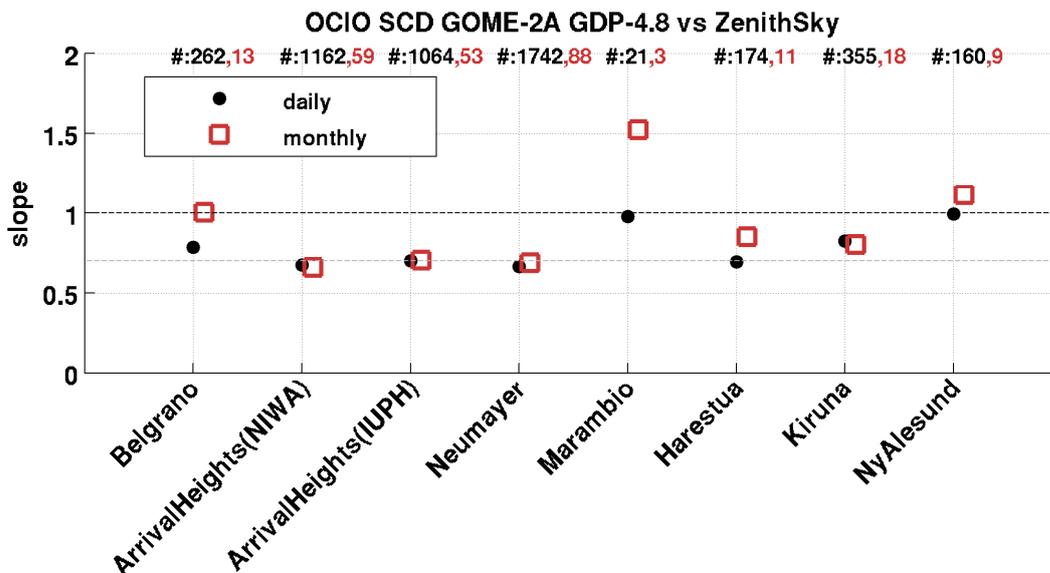


Figure C.3.1 Latitudinal overview of the linear regression slopes at each station between OCIO column data reported by (a)GOME-2A, (b) GOME-2B and by the ground-based zenith-sky DOAS spectrometers. The numbers in the upper part of the panel are the number of points for the comparison.

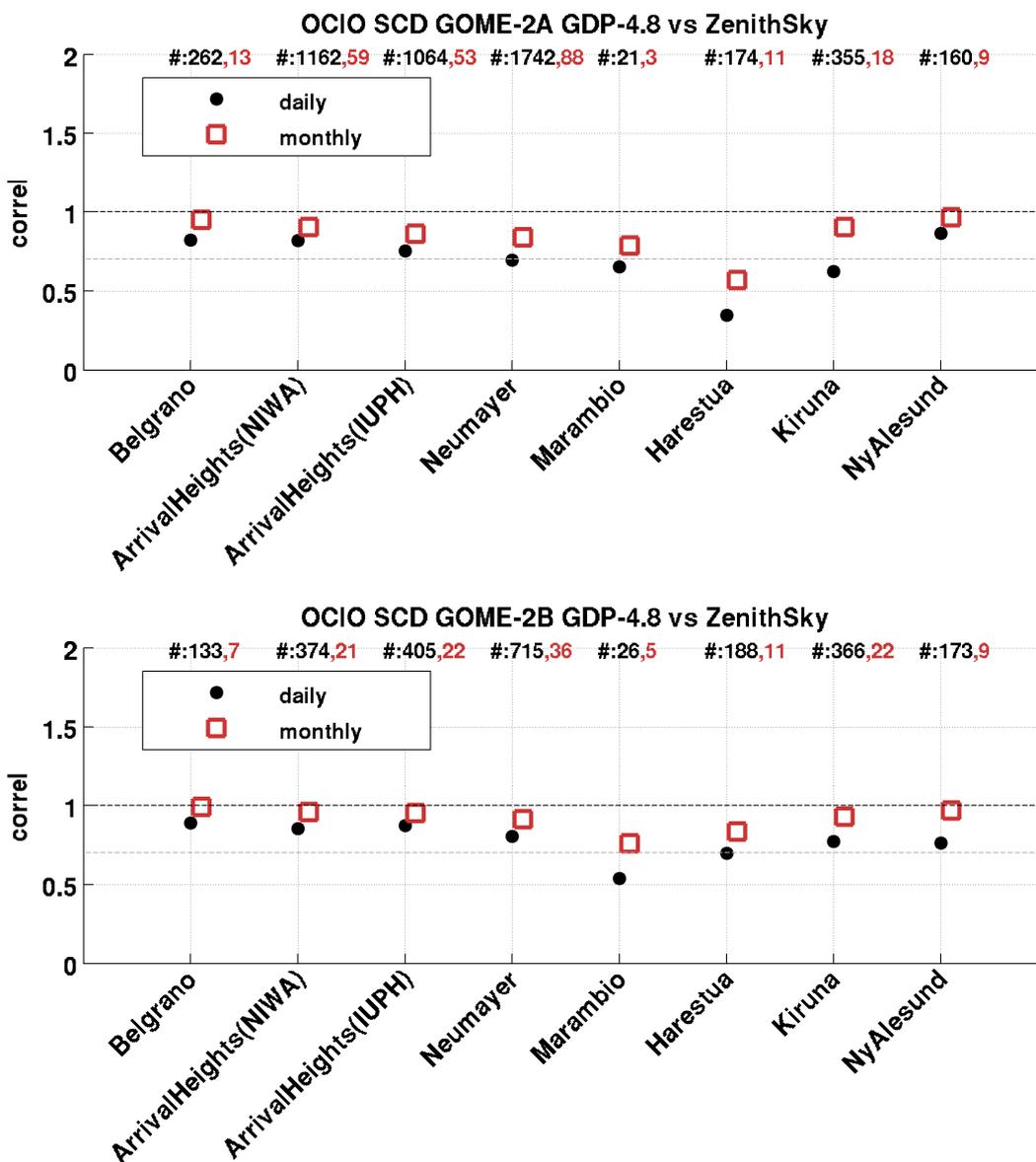


Figure C.3.2 Latitudinal overview of the correlation coefficient at each station between OCIO column data reported by (a)GOME-2A, (b) GOME-2B and by the ground-based zenith-sky DOAS spectrometers. The numbers in the upper part of the panel are the number of points for the comparison.

Table E.2: Summary of the regression parameters between GOME-2A and B and zenith-sky OCIO SCDs studied in this report.

Daily mean comparisons	GOME-2A	GOME-2B
<u>NyAlesund</u>	2013-2015	2013-2015

Regression parameters	R = 0.86 S = 0.99 I = 1.8e13	R = 0.76 S = 0.89 I = 6.2e12
Differences [molec/cm ²]	bias all: 1.8e+13 bias JFM: 2.9e+13	bias all: 3.2e+12 bias JFM: 7.9e+12
<u>Kiruna</u>	2013-2016	2013-2016
Regression parameters	R = 0.62 S = 0.82 I = 2.8e13	R = 0.77 S = 0.86 I = 1.6e13
Differences [molec/cm ²]	bias all: 2.4e+13 bias JFM: 1.7e+13	bias all: 1.2e+13 bias JFM: 1.1e+13
<u>Harestua</u>	03/2010-03/2015	01/2013-03/2015
Regression parameters	R = 0.35 S = 0.70 I = 1.6e13	R = 0.70 S = 0.81 I = 3.5e12
Differences [molec/cm ²]	bias all: 1e+13 bias JFM: -6.6e+12	bias all: -2.8e+11 bias JFM: -4e+12
<u>Neumayer</u>	2007-2016	2013-2016
Regression parameters	R = 0.69 S = 0.67 I = -1.8e13	R = 0.80 S = 0.63 I = -1.4e13
Differences [molec/cm ²]	bias all: -3.4e+13 bias JAS: -4.2e+13	bias all: -3.7e+13 bias JAS: -6.9e+13
<u>Arrival Heights IUPH</u>	2007-2016	2013-2016
Regression parameters	R = 0.75 S = 0.70 I = -2.4e13	R = 0.87 S = 0.71 I = -1.2e13
Differences [molec/cm ²]	bias all: -3.6e+13 bias JAS: -5.3e+13	bias all: -2.5e+13 bias JAS: -5.5e+13
<u>Arrival Heights NIWA</u>	2007-2016	2013-2016
Regression parameters	R = 0.82 S = 0.67 I = -2.2e13	R = 0.85 S = 0.65 I = -7.3e12
Differences [molec/cm ²]	bias all: -4.3e+13 bias JAS: -8.6e+13	bias all: -3.2e+13 bias JAS: -8.5e+13
<u>Belgrano</u>	2011, 2015	2015
Regression parameters	R = 0.82 S = 0.79 I = -3.4e13	R = 0.89 S = 0.80 I = 1e13

Differences [molec/cm ²]	bias all: -4.8e+13, bias JAS: -3.3e+13	bias all: -4.8e+13, bias JAS: -8.4e+12
<u>Marambio within 200 km</u>	2015	2015
Regression parameters	R = 0.70 S = 0.94 I = -9e13	R = 0.78 S = 0.85 I = -4.5e13
Differences [molec/cm ²]	bias all: -9.9e+13 bias JAS: -5.2e+13	bias all: -6.6e+13 bias JAS: -3.9e+13
<u>Marambio within 50 km</u>	2015	2015
Regression parameters	R = 0.65 S = 0.98 I = -8.8e13	R = 0.54 S = 1.09 I = -7.3e13
Differences [molec/cm ²]	bias all: -9.2e+13 bias JAS: -3e+13	bias all: -6.1e+13 bias JAS: -3.3e+13

When considering all the stations together, and focusing only on the activated period (July-August-September in the Southern Hemisphere and January-February-March in the Northern Hemisphere), scatter plot of satellite versus ground-based data can be drawn, as in figures C.3.4 for GOME-2A and C.3.5 for GOME-2B. The correlation coefficients derived from the daily scatterplots are about ~0.71 for GOME-2A and ~0.87 for GOME-2B, while the regression slope is 0.58 for GOME-2A and 0.64 for GOME-2B. Again, these results are within the target accuracy of 50% and close to the optimal accuracy of 30% for GOME-2B.

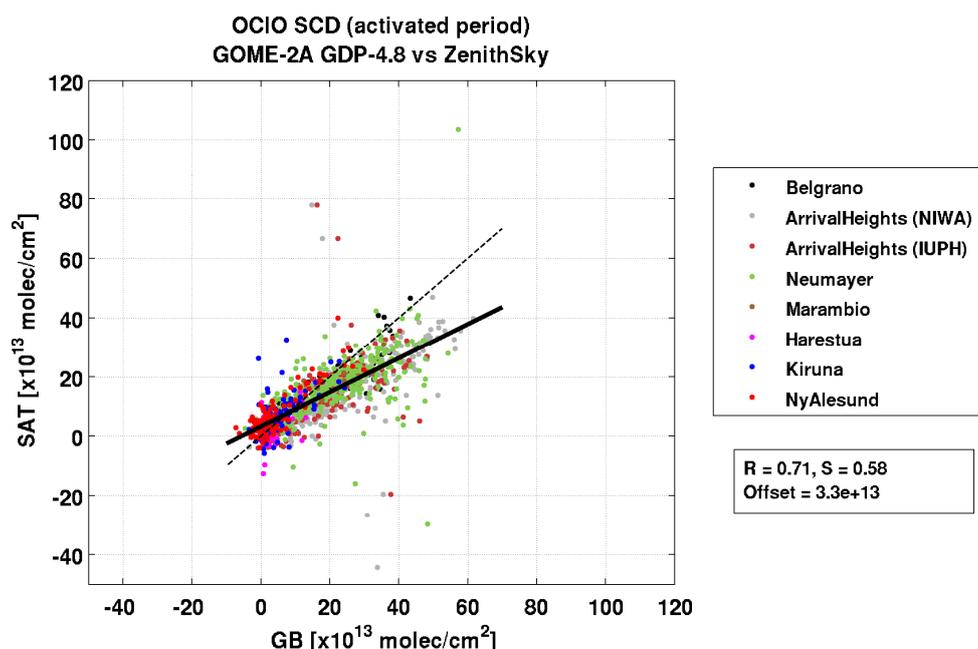


Figure C.3.4 Scatter plot between daily GOME-2A GDP 4.8 satellite data and ground-based data at the 8 stations included in the study, for the activated months (JAS for stations in the SH and JFM for stations in the NH).

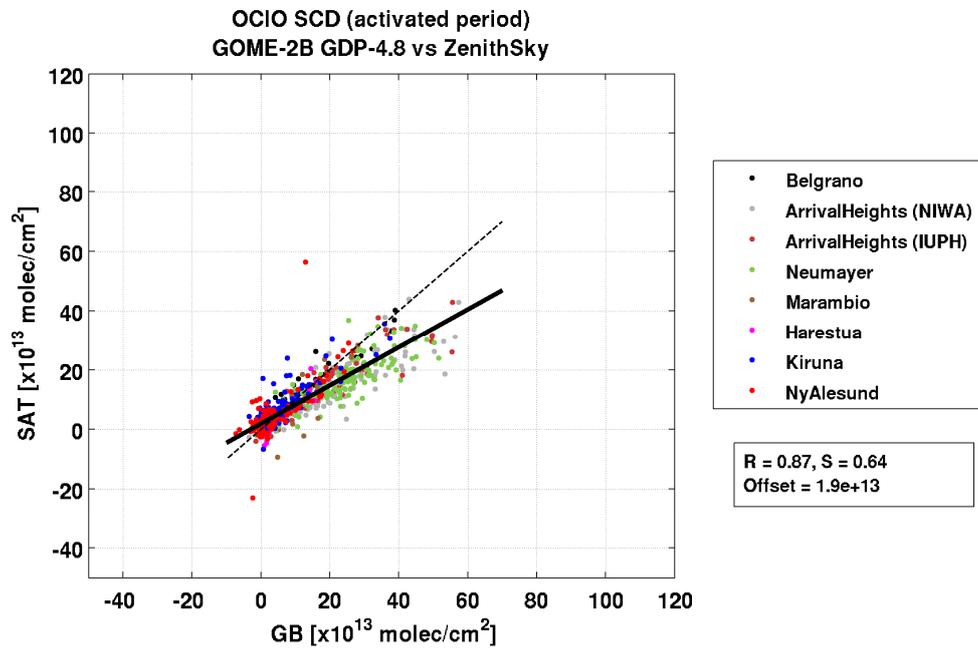
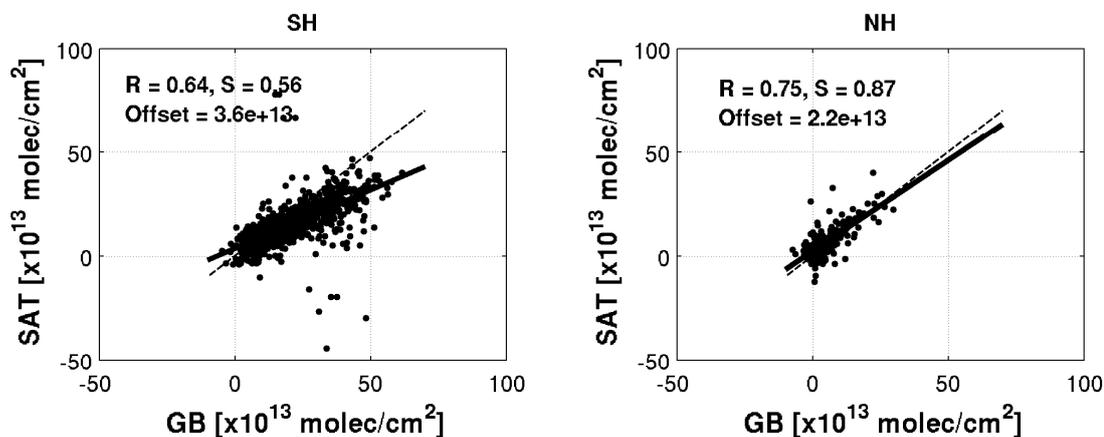


Figure C.3.5 Scatter plot between daily GOME-2B GDP 4.8 satellite data and ground-based data at the 8 stations included in the study, for the activated months (JAS for stations in the SH and JFM for stations in the NH).

If we separate these results by hemisphere, the slopes are 0.86/0.87 for the Northern Hemisphere and slightly smaller (0.56/0.62) for the Southern Hemisphere, as seen in figure C.3.6.

OCIO SCD (activated period)
GOME-2A GDP-4.8 vs ZenithSky



OCIO SCD (activated period)
GOME-2B GDP-4.8 vs ZenithSky

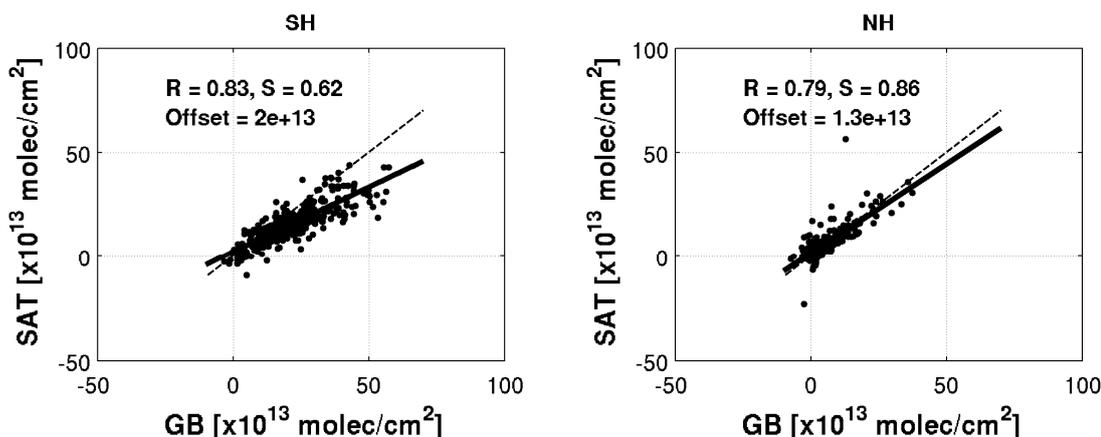


Figure C.3.6 Scatter plot between daily GOME-2A and -B GDP 4.8 satellite data and ground-based data at the 8 stations included in the study, for the activated months (JAS for stations in the SH and JFM for stations in the NH), separated by hemisphere.

From the previous figures and previous section, we can conclude that:

- Variations of the OCIO column, from day-to-day fluctuations to the annual cycle, are captured consistently by all measurement systems.
- Over the Southern Hemisphere both GOME-2 instruments report lower values than zenith-sky DOAS spectrometers, by about 40% while in the Northern Hemisphere the under-estimation is only about 15% when considering all stations together and focusing only on the chlorine activation period.

D. CONCLUSIONS

This document reports on the validation of AC SAF GOME-2 A and B OCIO column dataset products retrieved at DLR with versions 4.8 of the GOME Data Processor (GDP).

We investigated the quality of the GOME-2A (2007-2016) and GOME-2B (2012-2016) OCIO GDP 4.8 slant columns datasets by comparing them to ground-based measurements at a selection of eight DOAS zenith-sky stations located in the Arctic and Antarctic regions: Eureka (80°N), NyAlesund (79°N), Kiruna (68°N), Harestua (60°N), Marambio (64°S), Belgrano (78°S), Neumayer (71°S) and Arrival Heights (78°S). OCIO spectral analyses have been performed by each data provider using fixed noon spectra recorded at low SZA in the absence of chlorine activation. At each station, daily comparisons have been performed by selecting satellite and ground-based SCD data pairs corresponding to similar SZA conditions, and by making the assumption that the AMF is similar for satellite and ground-based measurement in these geometries. This assumption has been shown to be valid to within +/- 4% (Oetjen et al., 2011).

Daily and monthly mean OCIO SCD time-series show that satellite and ground-based observations agree well at all stations, both in terms of seasonal and inter-annual variabilities. GOME-2A tends to be more noisy especially after 2013, which is likely to be related to possible degradation effects.

Daily scatterplots based on data selected within activated periods give correlation coefficients of ~0.71 for GOME-2A and ~0.87 for GOME-2B, and regression slopes are of 0.58 for GOME-2A and 0.64 for GOME-2B. These results fulfill accuracy requirements for OCIO, as stated in the Product Requirement Document, i.e.: a target accuracy of 50% and an optimal accuracy of 30%.

There appears to be a hemispheric dependence of the agreement, with larger differences compared to zenith-sky DOAS spectrometers in the Southern Hemisphere (about 40%). In the Northern Hemisphere the under-estimation is significantly smaller (about 15%). This behavior was assessed considering all stations and focusing only on chlorine activated periods.

E. REFERENCES

E.1. Applicable documents

- [ATBD] Algorithm Theoretical Basis Document for GOME-2 Total Column Products of Ozone, NO₂, BrO, SO₂, H₂O, HCHO, OCIO and Cloud Properties (GDP 4.8 for AC SAF OTO and NTO), SAF/AC/DLR/ATBD/01, Iss. 3/A, Rev. 2.0, Valks, P., et al., 2017.
- [PUM] Product User Manual for GOME-2 Total Column Products of Ozone, NO₂, BrO, HCHO, SO₂, H₂O, OCIO and Cloud Properties, SAF/AC/DLR/ATBD/01, Iss. 3/A, Rev. 2.0, Valks, P., et al., 2017.
- [PRD] AC SAF Product Requirements Document, SAF/AC/FMI/RQ/PRD/001/Rev. 1.0, D. Hovila, S. Hassinen, D. Loyola, P. Valks, J., S. Kiemle, O. Tuinder, H. Joench-Soerensen, F. Karcher, 2017.
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E.2 Peer-reviewed articles

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