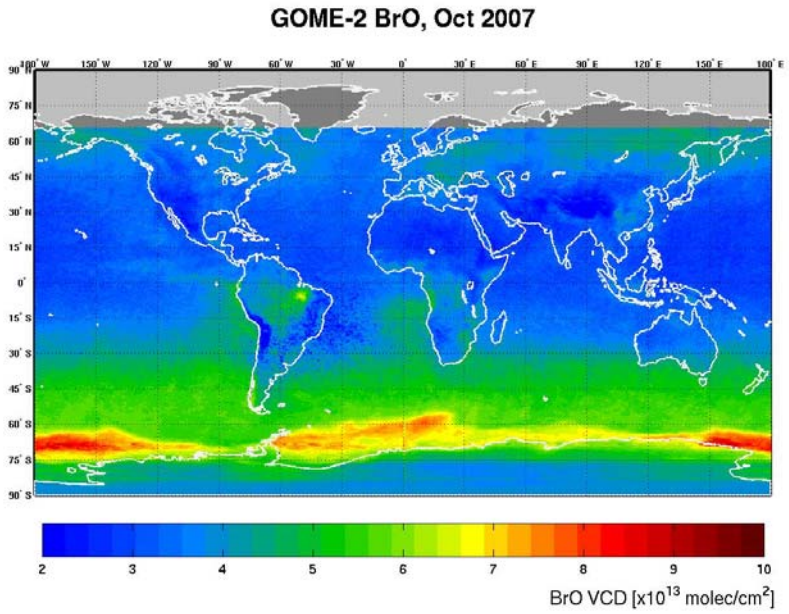
O3M SAF VALIDATION REPORT

Validated products:

Identifier	Name	Acronym
O3M-08	Offline Total BrO	OTO/BrO



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Reporting period: June 2007 – June 2008

Input data versions: GOME-2 Reprocessed Data-set L1B-R1, processor version 4

Data processor versions: GDP 4.3, UPAS version 1.3.0

Validation of GOME-2 GDP 4.3 BrO total columns – ORR B2

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ACRONYMS AND ABBREVIATIONS

AMF	Air Mass Factor, or optical enhancement factor
BIRA-IASB	Belgian Institute for Space Aeronomy
BrO	bromine monoxide
DLR	German Aerospace Centre
DOAS	Differential Optical Absorption Spectroscopy
ENVISAT	Environmental Satellite
ERS-2	European Remote Sensing Satellite -2
ESA	European Space Agency
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FMI	Finnish Meteorological Institute – Arctic Research Centre
GB-DOAS	Ground-based DOAS instruments
GDP	GOME Data Processor
GOME	Global Ozone Monitoring Experiment
H_2O	Water Vapor
IMF	Remote Sensing Technology Institute
NDACC	Network for the Detection of Atmospheric Composition Change
O3M-SAF	Ozone and Atmospheric Chemistry Monitoring Satellite Application Facility
OMI	Ozone Monitoring Instrument
ROCINN	Retrieval of Cloud Information using Neural Networks
SCD	Slant Column Density
SCIAMACHY	Scanning Imaging Absorption spectroMeter for Atmospheric CHartography
SZA	Solar Zenith Angle
TEMIS	Tropospheric Emission Monitoring Internet Service
UPAS	Universal Processor for UV/VIS Atmospheric Spectrometers
VCD	Vertical Column Density
WMO	World Meteorological Organization

A. INTRODUCTION

A.1. Scope of this document

The present document reports on the verification and initial validation of MetOp-A GOME-2 BrO total column data over the June 2007 - June 2008 time period, produced by the GOME Data Processor (GDP) version 4.3 operated at DLR on behalf of EUMETSAT. This report includes verification work performed using the BIRA-IASB scientific retrieval tool synchronized on the GDP settings, as well as comparisons with SCIAMACHY and ground-based measurements. The aim is to investigate whether the GOME-2 BrO total column product fulfill the user requirements in terms of accuracy, as stated in the Product Requirements Document (PRD - Threshold accuracy: 50%; Target accuracy: 30%; Optimal: 20%).

A.2. Preliminary notes

BrO total columns as generated from GDP version 4.3 represent a new GOME-2 product, generated within the GDP operational environment system at DLR.

The aim of the present document is first to report on the status of the verification of the GOME-2 BrO column against a synchronised scientific algorithm available at BIRA. For this exercise, BrO retrieval settings selected by DLR scientists for GDP version 4.3 are being used. The consistency of this BrO product is then explored by performed various comparisons with existing correlative data sets, including scientific data sets from SCIAMACHY. Ground-based BrO column measurements available for the stations at Harestua in Norway and Lauder in New-Zealand are also used in an attempt to further document the geophysical consistency of the GOME-2 BrO product.

It should be note here that improvements have been made in the BrO column retrieval for both the satellite instruments GOME-2 and SCIAMACHY and for the ground-based DOAS instruments, to resolve the apparent inconsistencies in the GOME-2 retrievals reported in the previous validation report for the ORR A3 (Van Roozendael et al., 2008a). The algorithm improvements for the satellite and ground-based DOAS instruments are described in this document.

Reported validation studies were carried out at the Belgian Institute for Space Aeronomy (IASB-BIRA, Brussels, Belgium) and at DLR Remote Sensing Technology Institute (DLR-IMF, Oberpfaffenhofen, Germany) in the framework of EUMETSAT Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring (O3M-SAF)

A.3. Plan of this document

This document is divided in four main parts, addressing respectively the description of the retrieval settings applied for the BrO product, the verification of this product, comparisons against satellite data and comparisons against ground-based measurements at Harestua and Lauder. This is followed by concluding remarks and perspectives for future work.

A.4. Applicable O3MSAF Documents

[ATBD] Algorithm Theoretical Basis Document for GOME-2 Total Column Products of Ozone, NO_2, SO_2, BrO, H_2O, HCHO, OClO, tropospheric NO2 and Cloud Properties, DLR/GOME-2/ATBD/01/2B, Valks, P., Loyola D., Hao N., Rix M., Slijkhuis S., 2009.

[PUM] Product User Manual for GOME Total Column Products of Ozone, NO_2, SO_2, BrO, H_2O, HCHO, OClO, tropospheric NO2 and Cloud Properties, DLR/GOME/PUM/01, Rev. 2/B, Loyola D., Zimmer W., Kiemle S., Valks P., Emmadi S., 2009.

[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.

A.5. Technical information

GOME-2 product name	BrO total column (OTO/BrO)
Validation reporting period	June 2007 - June 2008
Level-2 processor version	GDP 4.3, UPAS version 1.3.0
Input GOME-2 Level-1B data	GOME-2 Reprocessed Data-set L1B-R1, processor version 4

B. SETTINGS FOR BRO COLUMN RETRIEVAL FROM GOME-2

B.1. Experience from ERS-2 GOME and SCIAMACHY

BrO columns have been retrieved from ERS-2 GOME and ENVISAT SCIAMACHY instruments and settings used for these two instruments are documented in the literature (e.g. Chance, 1998; Richter et al., 1998, 2002, Wagner and Platt, 1998; Van Roozendael et al., 1999, 2002, 2004; De Smedt et al., 2004). For the GOME instrument on ERS-2, BrO slant columns have been commonly derived in the wavelength interval from 344.7 to 359 nm, making use of the characteristic absorption structures of BrO in this region. This interval has been so far considered as optimal for BrO fitting from both satellite and ground-based observations (see e.g. Aliwell et al., 2002; Richter et al., 1998, 1999; Van Roozendael et al., 1998; Wagner and Platt, 1998) since spectral interferences with O_3, O_4, and HCHO are minimised in this region. In the case of SCIAMACHY however different settings had to be adopted, mainly due to the existence of strong polarisation features in the channel 2 of SCIAMACHY that cannot be eliminated by the polarization correction scheme implemented in the Level 0-1 processing. This polarization feature generates spurious interferences with the BrO spectral structures. To get rid of these polarization-related interferences, another fitting interval was adopted for SCIAMACHY displaced at shorter wavelengths in a region less affected by the polarization anomaly but still showing prominent BrO absorption features. It was shown that equally acceptable BrO columns could be retrieved from SCIAMACHY by including two absorption bands (336-347 nm) or three bands (336-351 nm). The SCIAMACHY BrO interval was generally found to produce BrO slant columns in good agreement with GOME (De Smedt et al., 2004; Van Roozendael et al., 2004), although a significant interference with HCHO absorption was noted. SCIAMACHY BrO maps also display systematic negative biases that correlate with orography, possibly due to unresolved spectral interferences with Ring or O_2-O_2.

B.2. Choice of BrO slant column settings for GOME-2

In an attempt to define a baseline for GOME-2 processing, the GOME and SCIAMACHY settings have been tested on GOME-2 spectra. As a result of the smaller pixel size of GOME-2 observations (approx. 40x80 km^2 instead of 40x320 km^2 for GOME) the noise on the individual GOME-2 BrO measurements was found to be significantly increased in comparison to GOME. On the basis of noise-driven considerations and test retrievals performed at DLR and BIRA, the SCIAMACHY fitting interval using three absorptions bands (336 – 351.5 nm) was found to represent an optimal for GOME-2 retrieval and was selected for the generation of a data set, which we now consider for evaluation.

Although, the noise level was found to be significantly reduced in the 336-351.5 nm interval in comparison with the GOME baseline (344.7-359 nm), the comparison of BrO columns retrieved from GOME-2 in both spectral regions also revealed systematic differences, in particular a tendency to produce lower BrO slant columns at shorter wavelengths(Van Roozendael et al., 2008a). In order to investigate the possible reasons of this difference in an attempt to reconcile BrO retrievals in both intervals, a series of sensitivity tests have been performed (Van Roozendael et al., 2008b). DOAS settings were varied in both intervals and the stability of the BrO slant columns was investigated. It was found that the retrieved BrO slant columns are more stable in the shorter wavelength interval. In particular it was found that in the longer wavelength range, BrO slant columns are highly sensitive to the choice of the reference laboratory cross-sections of both O_3 and O_4. According to our tests, a switch from our past baseline (O_3 cross-sections from Burrows et al., 1999 and O_4 cross-sections from Greenblatt et al., 1990) to an alternative choice of laboratory measurements, i.e. O_3 cross-sections from Brion et al. (1998) and O_4 cross-sections from Hermans et al. leads to significantly smaller BrO columns in better agreement with results obtained in the 336-351.5 nm interval.

The detailed DOAS settings used for GOME-2 BrO slant columns retrieval are given in Table1.

Table 1. DOAS settings used for GOME-2 BrO slant column verification

Fitting interval	336 – 351.5 nm
Sun reference	Sun irradiance from file
Wavelength calibration	Wavelength calibration of sun reference optimized by NLLS adjustment on convolved Chance and Spurr solar lines atlas
Absorption cross-sections	
- BrO	Fleischmann et al., 223°K
- NO_2	GOME FM3, 243°K
- Ozone	Brion et al. 1998, convolved at GOME-2 resolution, 218°K + 243°K
- O_2-O_2	Hermans et al.
- Ring effect	2 Ring eigenvectors generated using SCIATRAN
Polynomial	3rd order (4 parameters)
Intensity offset correction	Constant offset

In order to convert the retrieved BrO slant columns into vertical columns, Air Mass Factors (AMF) are calculated for each pixel. The AMFs are generated with the LIDORT 3.3 radiative transfer model in the GDP 4.3 environment, using pure stratospheric BrO profiles.

Figures 1 and 2 present examples of results for one day in October 2007 and the monthly mean for October 2007.

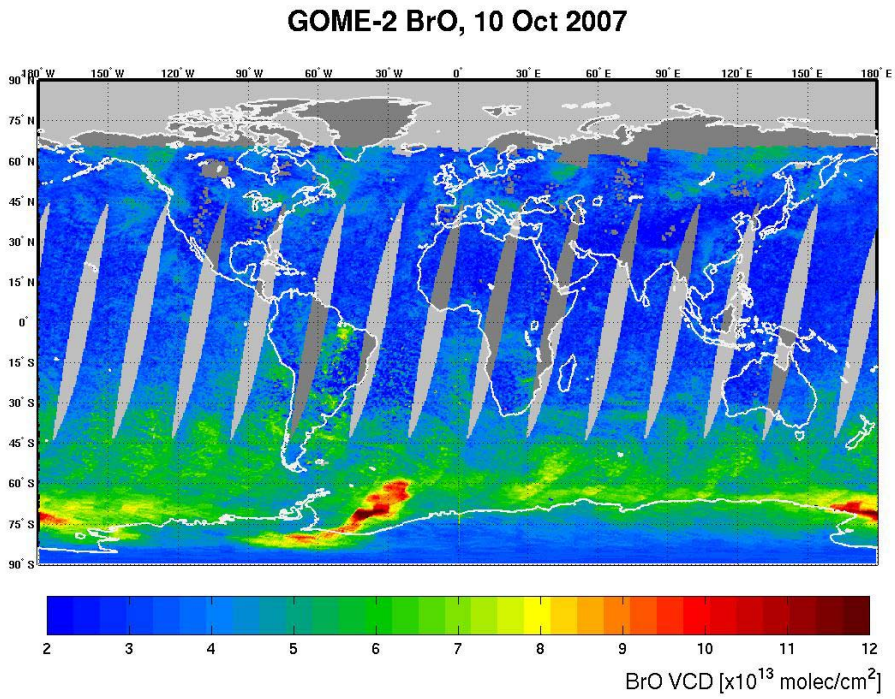


Figure 1. BrO vertical columns derived from GOME-2 nadir radiances for 10th October 2007 (using the baseline settings given in Table 1).

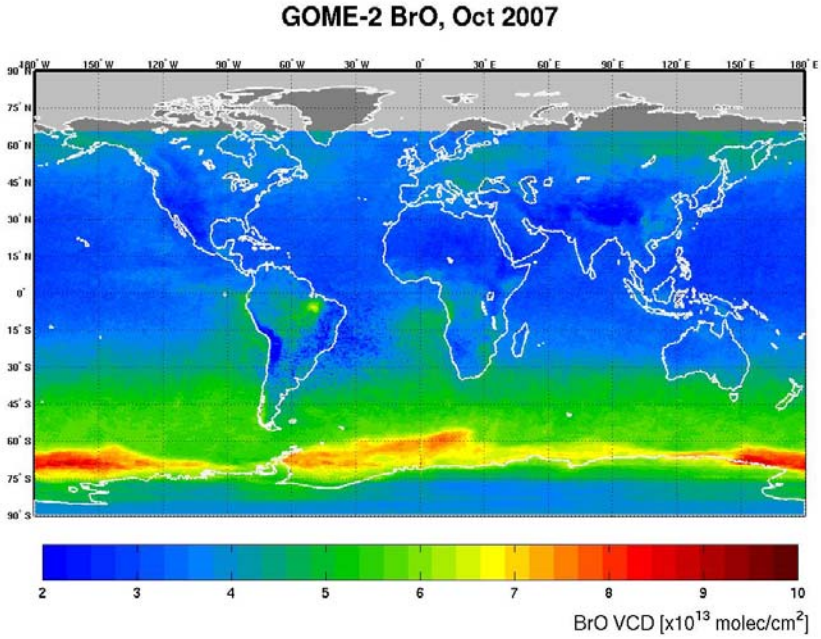


Figure 2. Monthly averaged of GOME-2 BrO vertical columns retrieved for October 2007 (using the baseline settings given in Table 1).

Note that the known interference between spectral signatures of BrO and HCHO result in BrO columns being positively biased over regions of large HCHO emissions (e.g. central Africa, southern America or eastern China).

In the following sections the consistency of the GDP 4.3 BrO column product is investigated from the point of view of (1) the verification (i.e. whether BrO retrievals performed with GDP 4.3 are consistent with scientific retrievals performed using same settings), (2) the comparison against another satellite instrument (SCIAMACHY), and (3) the comparison against independent ground-based observations from two stations of the NDACC network.

C. VERIFICATION OF BRO SLANT COLUMNS

For verification purposes, the retrieval software of BIRA-IASB was synchronised with the GDP 4.3 processor, using a common set of slant column retrieval settings, as documented in Table 1. Comparisons between the two processing systems were performed on a limited set of GOME-2 orbits. Results of these comparisons are illustrated in Figures 3. As can be seen, a good level of agreement was obtained, demonstrating the consistency between the two slant column fitting algorithms. The differences in BrO SCDs retrieved from GDP 4.3 processor and BIRA-IASB software show a small bias of -1 x 10^{12} molec/cm² and a standard deviation of 1 x 10^{13} molec/cm².

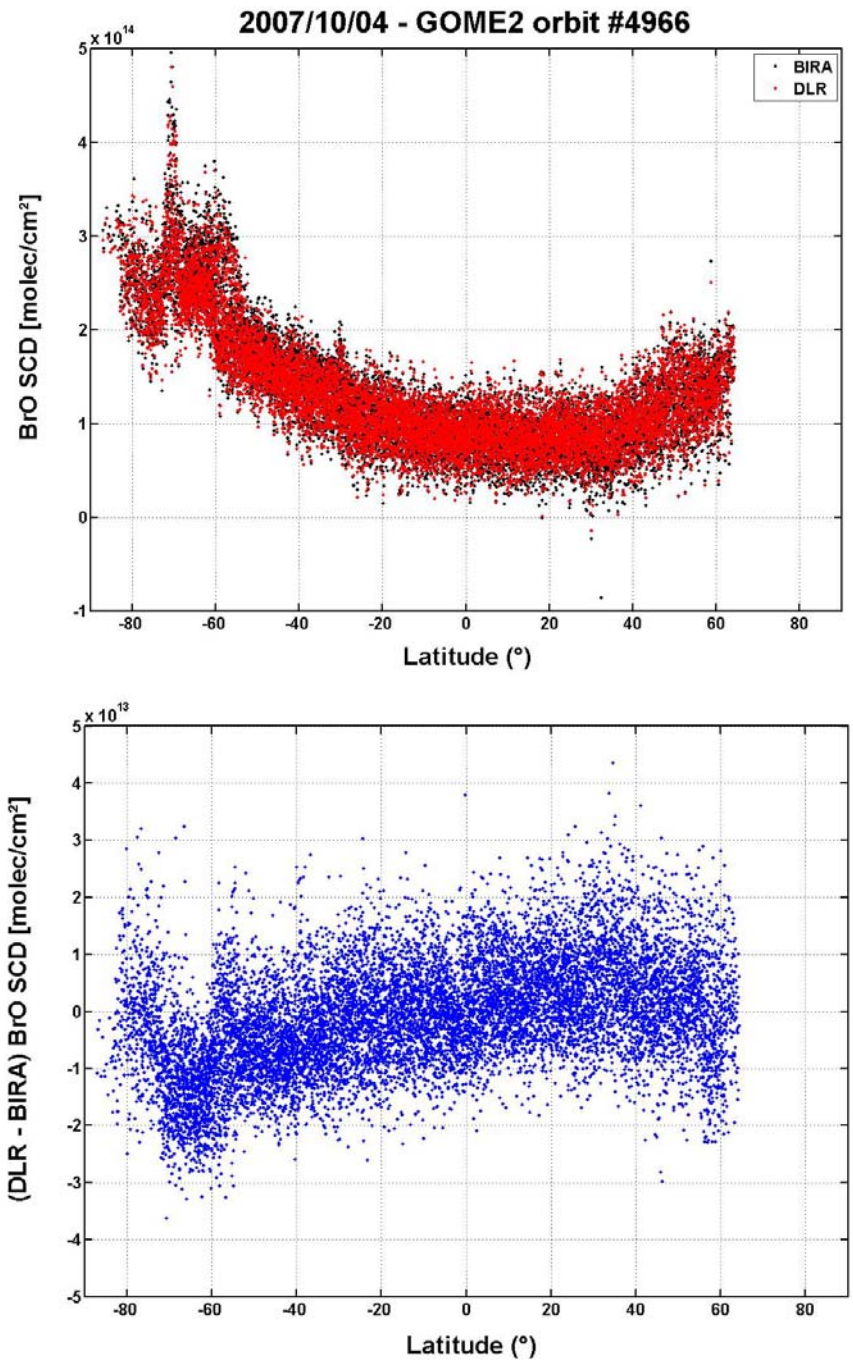


Figure 3 Comparison of BrO slant columns retrieved from GDP 4.3 and from the BIRA-IASB scientific algorithm. The lower plot corresponds to the difference between GDP 4.3 and BIRA-IASB BrO SCDs. DOAS settings were synchronized according to Table 1.

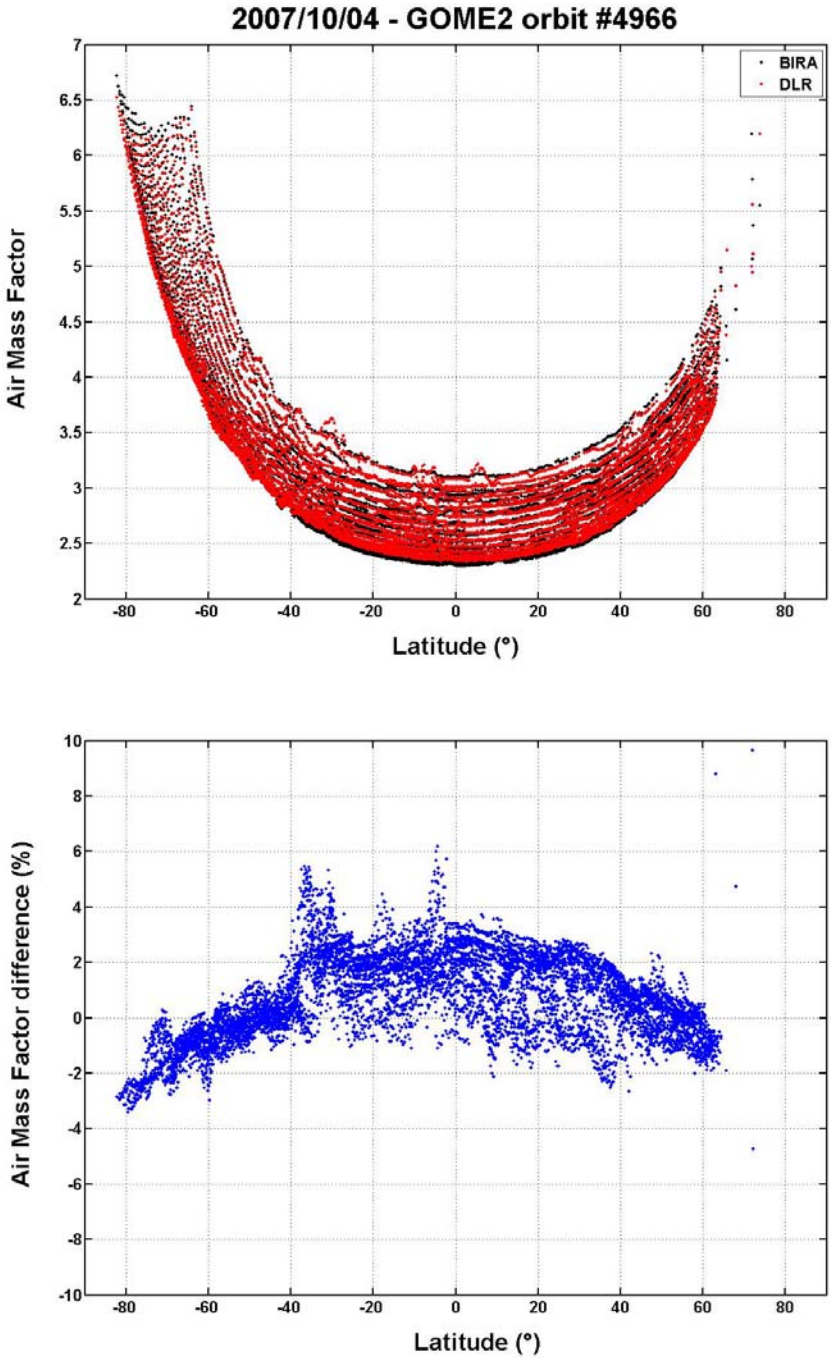


Figure 4 Comparison of BrO Air Mass Factors calculated from LIDORT (DLR) and DISORT (BIRA-IASB). The lower plot corresponds to the difference between LIDORT and DISORT BrO AMFs.

Additional verification has been made on the AMFs calculated in GDP 4.3. These AMFs have been compared with the AMFs calculated using the UVspec/DISORT package (Mayer and Kylling, 2005). The results are illustrated on Figure 4. Good agreement is found, both datasets showing consistent results as a function of latitude (or solar zenith angle) and viewing angles. The differences in BrO SCDs retrieved from GDP 4.3 processor and BIRA-IASB software show a small bias of +0.7% and a standard deviation of 1.5%.

Based on a limited number of orbits, we have also estimated the noise on the retrieved BrO slant and vertical columns. From the fitting results and the scatter of GOME-2 data, the noise on the BrO slant columns is in the range from 2.5 to 4.5 10^{13} molec/cm² for latitudes varying from the equator to the poles. This translates to ~25 to 35% of the total BrO vertical columns.

D. COMPARISON AGAINST SATELLITE DATA

BrO slant and vertical column amounts derived from SCIAMACHY instrument have been produced at BIRA-IASB as part of the DUP/DUE TEMIS service (www.temis.nl). This data set has been used here for comparison with GOME-2 retrievals from the GDP 4.3 data set. It should be noted that the SCIAMACHY data set was initially generated using the outdated BrO cross-section from Wahner et al. (1988). This cross-section suffers from inadequate spectral resolution, which results in a systematic overestimation of the BrO slant columns by approximately 20 %. Consequently the SCIAMACHY data set has been reprocessed with the BrO cross-section of Fleischmann et al. (2004), the same as used in the GOME-2 retrieval (but convolved at the spectral resolution of SCIAMACHY). In order to simplify the comparison process within the limited timeframe available for this study, we based our analysis on overpass files extracted by the DLR team for a number of ground-based correlative sites, as detailed in Table 2.

Table 2. List of overpass sites used for the comparison with SCIAMACHY

Station	**Latitude [°]**	**Longitude [°]**	**Altitude [m]**
Ny_Alesund	78.92	11.92	8
Scoresbysund	70.48	-21.97	17
Sodankyla	67.37	26.65	179
Salekhard	66.67	66.67	0
Jokioinen	60.82	23.48	103
Helsinki	60.32	24.97	56
Harestua	60.20	10.80	580
St_Petersburg	59.97	30.30	60
Zvenigorod	55.68	36.77	200
Hamburg	53.57	9.97	105
Leicester	52.62	-1.12	90
De_Bilt	52.10	5.18	15
Cabauw	51.97	4.93	10
Paris	48.85	2.35	50
Verrieres_Le_Buisson	48.76	2.24	0
Jungfraujoch	46.55	7.98	3450
Haute.Provence	43.91	5.75	580
Issyk Kul	42.62	76.97	1640
Thessaloniki	40.63	22.96	60
XiangHe	39.75	116.96	36
GSFC	38.99	-76.84	102
Table_Mountain	34.38	-117.68	2200
Sevilleta	34.35	-106.88	1477
Kanpur	26.45	80.35	142
Mussafa	24.37	54.47	10

Mukdahan	16.61	104.68	166
Djougou	9.71	1.68	430
Ilorin	8.32	4.34	350
Merida	8.24	-71.08	4765
Nairobi	-1.32	36.92	1624
La Reunion	-21.06	55.48	24
Sao_Paulo	-23.56	-46.73	865
Kerguelen	-49.35	70.25	2
Dumont_D'Urville	-66.67	140.02	40

GOME-2 and SCIAMACHY BrO columns have been extracted above each site according to measurement periods available from the different data sets. In order to provide a meaningful temporal perspective, time-series of monthly averaged BrO columns have been plotted for comparison over the time period from June 2007 until June 2008. In the case of SCIAMACHY, simple geometrical AMFs were used for the slant to vertical column conversions. It was verified that under these conditions, the GDP 4.3 AMFs are close to geometrical AMFs within a few percents. Results from the SCIAMACHY and GOME-2 comparisons are represented in Figure 5 for a representative selection of sites.

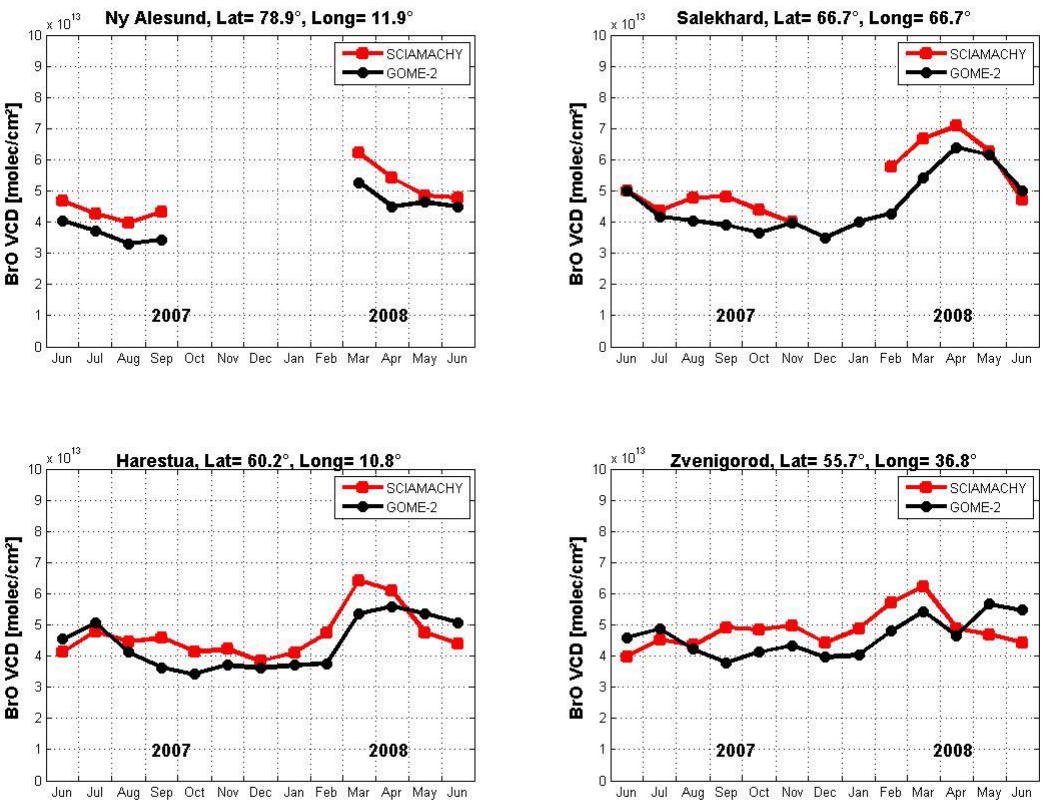


Figure 5. Comparison of time-series of monthly averaged BrO vertical columns retrieved from SCIAMACHY and GOME-2 over the June 2007- June 2008 period, at a number of ground-based sites.

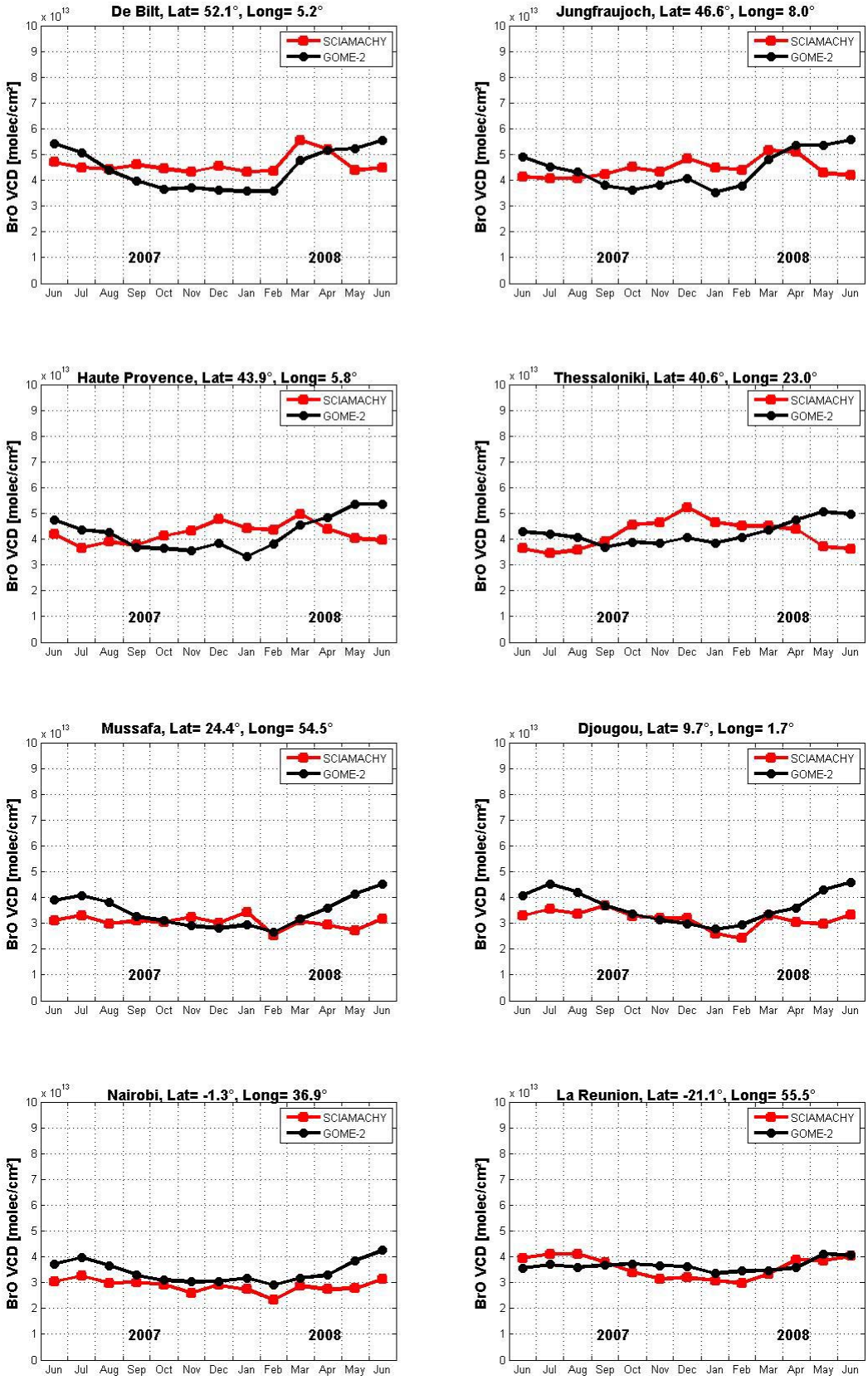


Figure 5. Continued

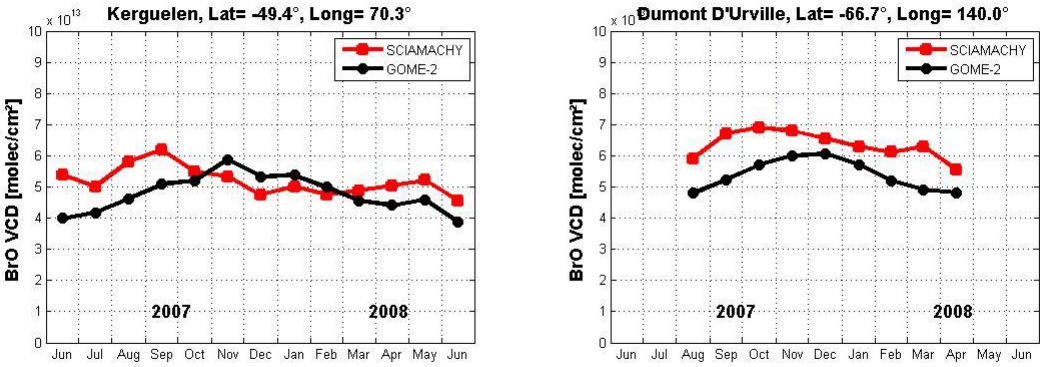


Figure 5. Continued

In generally, the GOME-2 and SCIAMACHY BrO columns show a fairly good agreement. However, as can be seen in Figure 5, the GOME-2 retrieval generally gives lower BrO columns than the SCIAMACHY data at high latitude sites of both hemispheres. At mid-latitudes, the general agreement is generally better although the seasonal patterns seem to be different. In the tropics and equatorial belts, the average level is highly consistent for these two data sets.

In Figure 6, all coincident monthly average BrO VCD values are compared in a correlation plot. The column-dependency of the differences (reaching 20 percents for the largest columns) is more clearly depicted in Figure 7, where relative differences with respect to SCIAMACHY are expressed as a function of the BrO VCD. Note that the relative differences between GOME-2 and SCIAMACHY BrO VCDs are within the PRD threshold, target and optimal accuracies respectively for 100%, 93.5% and 75.4% of the data.

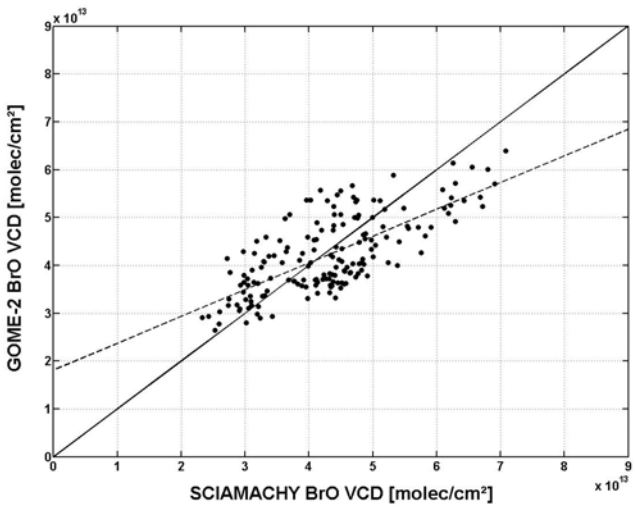


Figure 6. Correlation between BrO VCD retrieved from GOME-2 and SCIAMACHY (correlation coefficient: 0.71). The dashed line is the linear regression line (slope: 0.56, intercept: 1.8 10^{13} molec/cm²). The solid line represents the reference line of slope equal to unity

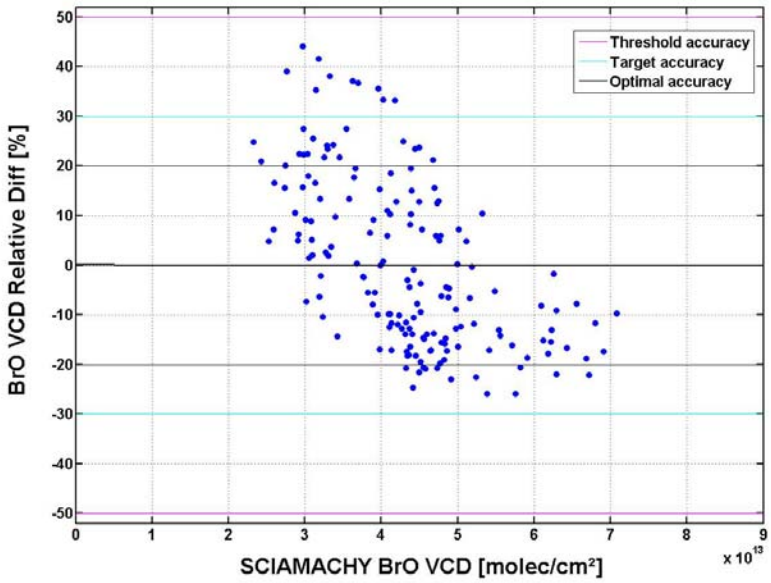
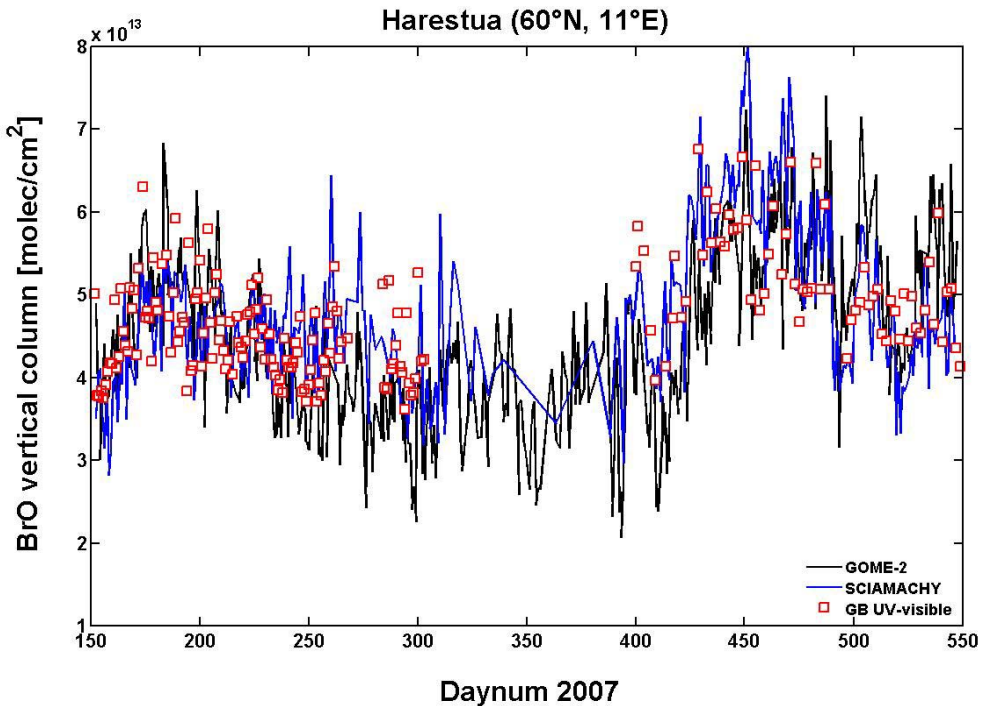


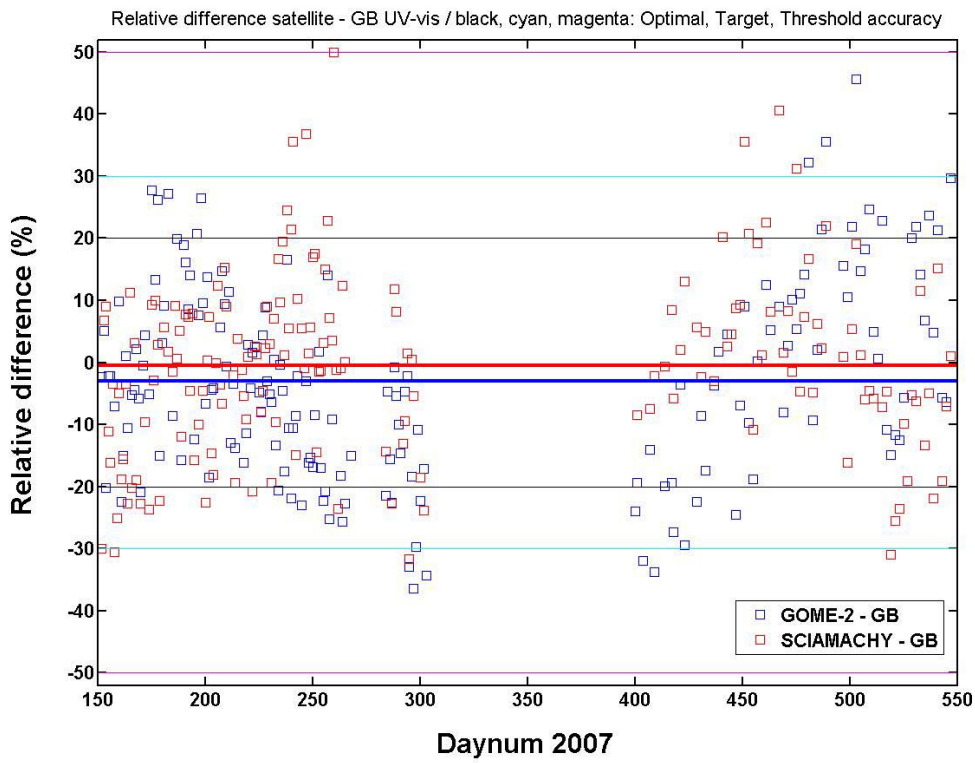
Figure 7. Relative difference in BrO VCD between GOME-2 and SCIAMACHY plotted as a function of SCIAMACHY BrO VCD.

E. COMPARISON AGAINST GROUND-BASED MEASUREMENTS

Ground-based zenith-sky UV-visible observations have been continuously performed at the NDACC station of Harestua, Norway since 1998 as well as in Lauder, New-Zealand since 1995. The instruments consist of zenith-sky looking grating spectrometers using cooled photodiode-array detectors. Spectral range and resolution are optimised for BrO measurements in the 330–360 nm. Total, stratospheric and tropospheric BrO columns are retrieved from measured slant columns using a profiling algorithm based on the optimal estimation method, as described in Hendrick et al. (2007). The sensitivity of the zenith-sky observations to the tropospheric BrO detection is increased by using for the spectral analysis a fixed reference spectrum corresponding to clear-sky noon summer conditions. The use of a photochemical box-model optimised for bromine chemistry embedded inside the inversion tool allows performing retrievals at any solar zenith angle, therefore allowing for appropriate photochemical matching with satellite observations.

In order to provide an independent reference, BrO total columns derived from latest versions of the ground-based measurements have been compared to GDP 4.3 BrO columns for the period from June 2007 until June 2008. The GOME-2 columns show a good agreement with ground-based results at Harestua and Lauder, as displayed in Figures 8 and 9. We estimate a bias and standard deviation respectively of (1) -3% and 16% at Harestua and (2) 2.5% and 12% at Lauder. These results are in contrast with those reported in the previous validation report for the ORR-A3 (Van Roozendael et al., 2008a) and reflect progress recently made in the evaluation of ground-based measurements now available at an increasing number of sites. Note that the relative differences between GOME-2 and ground-based BrO VCDs are within the PRD threshold, target and optimal accuracies respectively for 100%, 95.3% and 75.5% of the data at Harestua and for 100%, 98.1% and 89.7% of the data at Lauder. The SCIAMACHY data are also compared to our ground-based data set in Figures 8 and 9. The SCIAMACHY columns are generally also in fair agreement with the ground-based observations although they show a tendency to slightly overestimate the BrO columns at Lauder by about 17 %.


Harestua (60°N, 11°E)
x 10^13
BrO vertical column [molec/cm^2]
Daynum 2007
GOME-2
SCIAMACHY
GB UV-visible


Relative difference satellite - GB UV-vis / black, cyan, magenta: Optimal, Target, Threshold accuracy
Relative difference (%)
Daynum 2007
GOME-2 - GB
SCIAMACHY - GB

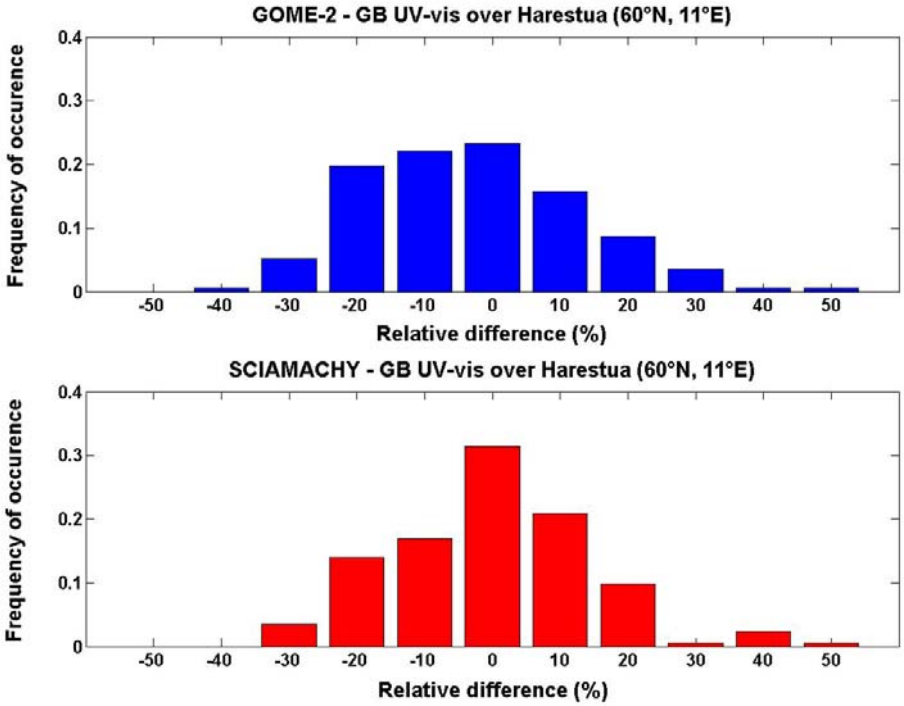
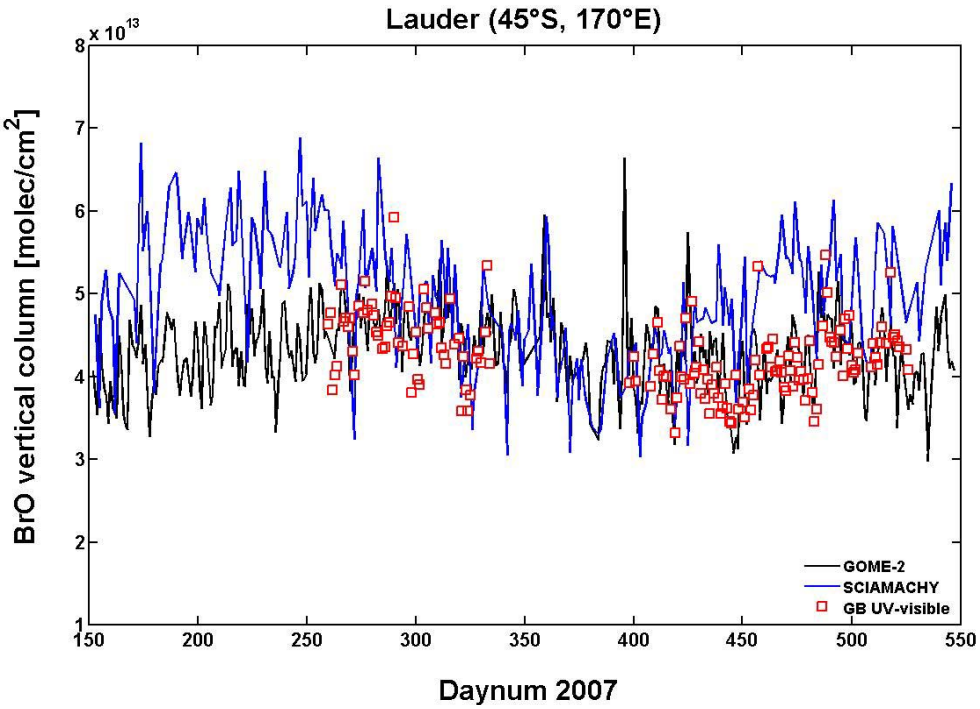


Figure 8. Comparison of BrO total columns retrieved from GOME-2, SCIAMACHY and from ground-based UV-visible measurements at the Harestua station (data originators: F. Hendrick and M. Van Roozendael).



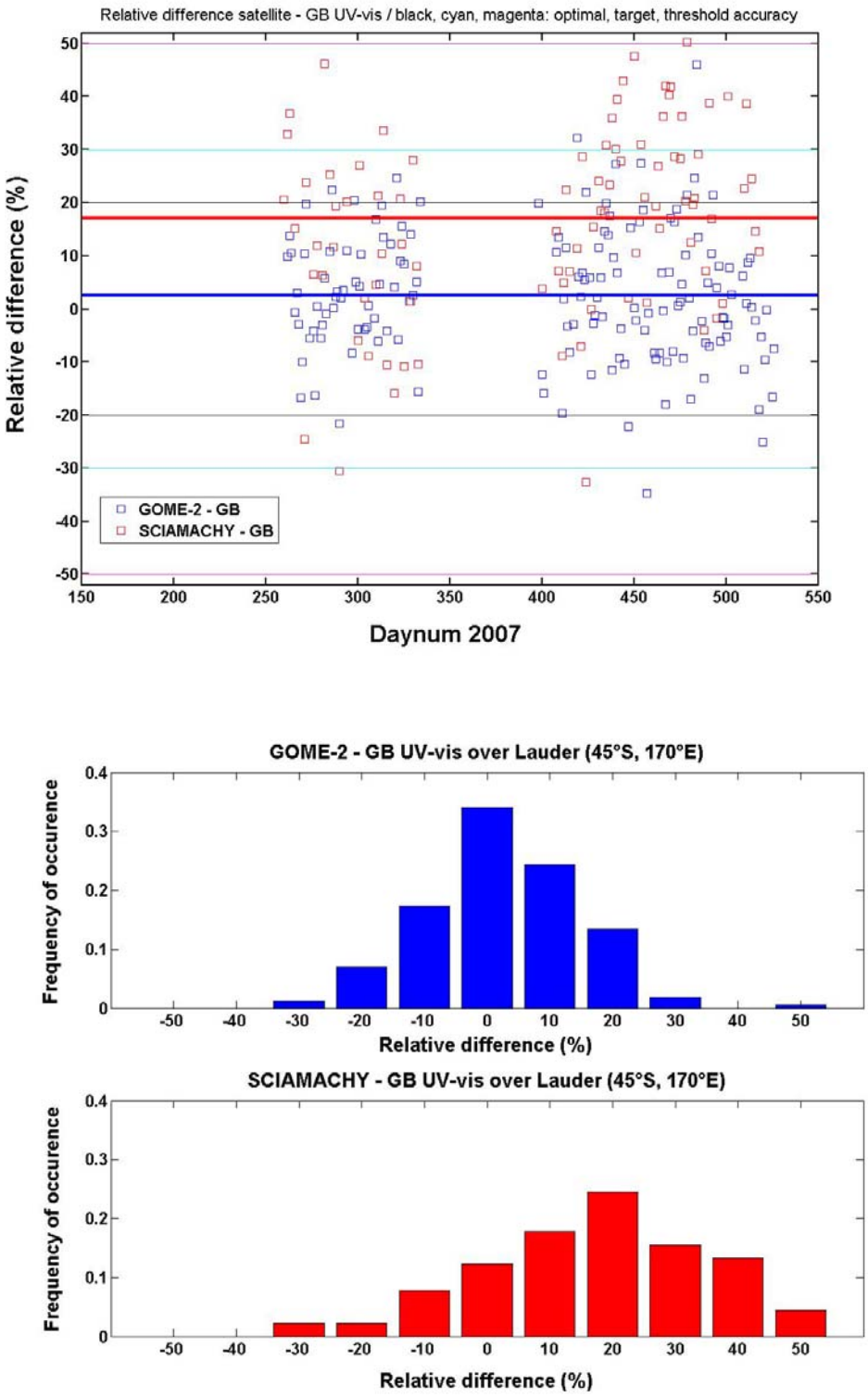


Figure 9. Comparison of BrO total columns retrieved from GOME-2, SCIAMACHY and from ground-based UV-visible measurements at the Lauder station (data originators: Paul Johnston and F. Hendrick).

F. CONCLUSIONS

As part of this validation report, the verification and validation of the GOME-2 total BrO product has been addressed, based on tools available at BIRA-IASB.

GOME-2 BrO vertical columns have been evaluated using (1) scientific retrievals based on the GDOAS tool and (2) comparisons with correlative data sets from SCIAMACHY and from ground-based zenith-sky measurements. The fitting interval 336-351.5 nm previously used for SCIAMACHY retrievals has been selected as baseline for BrO slant column retrieval in GDP 4.3. This interval has been found to minimize the noise on the GOME-2 BrO columns. The previous validation report for the ORR-A3 (Van Roozendael et al., 2008a) suggested that GOME-2 BrO slant columns tend to be underestimated when retrieved in this interval compared to GOME interval 345-359 nm. In order to resolve the apparent inconsistency, additional sensitivity tests have been performed to explore the stability of BrO slant column fit results in both fitting ranges. It is found that retrievals in the longer wavelength range (GOME interval) are more sensitive to uncertainties in O_3 and O_4 absorption cross-sections. A switch from our past baseline (O_3 cross-sections from Burrows et al., 1999 and O_4 cross-sections from Greenblatt et al., 1990) to an alternative choice of laboratory measurements, i.e. O_3 cross-sections from Brion et al. (1998) and O_4 cross-sections from Hermans et al. leads to significantly smaller BrO columns in better agreement with results obtained in the 336-351.5 nm interval. The stability of the DOAS fits in the 336-351.5 nm wavelength regions provides further evidence of the reliability of these retrievals.

For verification purpose, the GDOAS and GDP 4.3 retrieval tools were synchronized until a good level of agreement was found confirming the reliability of the GDP for BrO slant column fitting and for the calculation of air mass factors. The difference between GOME-2 and SCIAMACHY data show a moderate column-dependent pattern. The bias is found to be largest a high latitude reaching -13 % in average for BrO columns larger than $5x10^{13}$ molec/cm^2. The bias reaches +13% in average for BrO columns below $5x10^{13}$ molec/cm^2 at mid- and tropical latitudes.

Additional comparisons using latest versions of available ground-based DOAS measurements at two stations of the NDACC (Harestua, Norway and Lauder, New Zealand) further consolidate the GOME-2 retrievals with bias and standard deviation of the column differences kept in the range of +/- 3% and 16%, respectively. These results are in contrast with those reported in the previous validation report for the ORR-A3 (Van Roozendael et al., 2008a) and reflect progress recently made in the evaluation of ground-based measurements now available at an increasing number of sites.

Based on the validation with ground-based measurements and the comparisons with correlative SCIAMACHY data, we concluded that the current GOME-2 GDP 4.3 BrO column product already fulfill the user requirements and can be declared as fully operational.

For longer term validation, the currently expanding ground-based BrO monitoring capabilities will be further exploited. In particular the growing interest for the study of polar bromine emissions will lead to extension of ground-based MAXDOAS networks in polar regions.

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