INTEGRATED TRACE GAS VALIDATION AND QUALITY ASSESSMENT SYSTEM FOR THE EUMETSAT POLAR SYSTEM

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Abstract

In the framework of EUMETSAT's Satellite Application Facility on Ozone and Atmospheric Chemistry Monitoring (O3M-SAF), the second phase of the Continuous Development and Operations Project (CDOP-2) started in March 2012 with the aim to deliver operational GOME-2 and IASI data products of well characterized precision, accuracy and stability matching the needs of a large community of Users. The validation of new data products and the continuous monitoring of the quality of operational data sets are essential activities in the O3M-SAF. For minor trace gases, validation and Quality Assessment (QA) activities are coordinated at BIRA-IASB. During the first phase of CDOP, an end-to-end validation approach has been designed and demonstrated for GOME-2 NO_2 total and tropospheric column measurements. In compliance with international QA/QC standards, the idea is to evaluate independently all critical individual components of the level-1-to-2 retrieval chain. Evaluations are carried out by means of a suite of correlative observations performed by complementary ground-based and satellite instruments supported by radiative transfer and chemical-transport modelling tools. For CDOP-2, this precursor trace gas validation system will be significantly enhanced to cover a number of additional gases measured by the GOME-2 and IASI sensors (NO_2, BrO, H_2CO, SO_2, glyoxal, HNO_3 and OClO) on board of the three EUMETSAT MetOp platforms. A validation web portal will be set up, to report on the validation of new data products and on the continuous QA of operational products. Validation and QA will be based on a number of sources of ground-based correlative measurements, including remote-sensing zenith-sky, direct sun and MAXDOAS spectrometers, and FTIR instruments from selected NDACC stations. In addition, validation activities will include satellite-to-satellite comparisons relying on well-documented data sets from the GOME, SCIAMACHY and OMI instruments.

We present the concept of the system and illustrate its capabilities for NO_2, BrO and H_2CO validation using high-quality MAXDOAS measurements in Beijing/Xianghe (China), OHP (South of France) and Uccle (Belgium).

1. THE CDOP-2 PROJECT

In the framework of O3M-SAF CDOP-2 project, started in March 2012, BIRA-IASB coordinates the validation and Quality Assessment (QA) activities for minor trace gases. A full validation exercise is essential for new products before reaching operational status (e.g., development of new gases and application of the products to Metop-B), while the QA consists of regular online monitoring of operational products, in order to ensure their stability, including both internal verification by the developer institutes and regular comparisons to correlative datasets, performed by the validation groups. A validation web portal will be set up at BIRA-IASB, to regularly report validation and QA results for minor trace gases, such as NO_2, BrO, H_2CO, SO_2, glyoxal, HNO_3 and OClO.

Based on the experience developed during CDOP-1, an "end-to-end" approach has been developed to evaluate independently all critical components of the level-1-to-2 retrieval chain, using correlative observations performed by ground-based and satellite instruments. Satellite-to-satellite comparisons include GOME, SCIAMACHY and OMI instruments, while from the ground we focus on NDACC/BIRA stations (see Figure 1) that are equipped with remote-sensing zenith-sky, direct sun and MAXDOAS spectrometers and FTIR instruments. In a later stage, the idea is to expand the network to a larger number of instruments from the NDACC network. This will benefit from efforts done in the NORS project (Demonstration **N**etwork **O**f ground-based **R**emote **S**ensing Observations in support of the

GMES Atmospheric Service, http://nors.aeronomie.be/) to harmonize, automatize and bring operational level within the NDACC network.

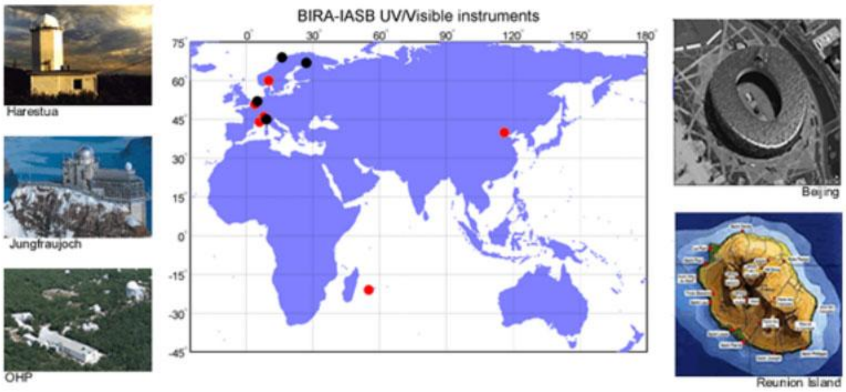

Figure 1: **Illustration of the BIRA-IASB instruments locations. Zenith-sky instrument are present in Harestua (Norway) since 1998 and in Jungfraujoch (Switzerland) since 1990. MAXDOAS instruments are measuring in OHP (South of France) since 2002, in Jungfraujoch since 2010 and in and close to Beijing (China) since 2008. FTIR measurements have been also performed at Reunion Island (Indian Ocean) since 2002.**

2. VALIDATION ACTIVITIES: NO_2

The validation of NO_2 was one of the main tasks of BIRA-IASB in CDOP-1 and the results can be found in Pinardi et al., 2011. This work is continued and further extended in CDOP-2. Here, we illustrate several aspects of this validation, like: (a) the end-to-end method, illustrated hereafter above OHP, (b) direct comparison of total/stratospheric columns with independent ground-based NDACC zenith-sky data, and (c) direct comparison of tropospheric columns with independent ground-based MAXDOAS data from BIRA-IASB stations.

2.1 End-to-end method illustrated above OHP

The NDACC station at Observatoire de Haute Provence (OHP, 44°N, 5.7°E) has been used in CDOP-1 to test and set up a method for the validation of GOME-2 GDP tropospheric NO_2 (Pinardi et al., 2010, Pinardi et al., 2011). The idea is to focus on the verification and comparison of the different elements of the L1-to-L2 retrieval chain, i.e.:

- Slant columns, by testing the operational algorithm on other datasets (e.g., GOME and SCIAMACHY) and on other state-of-the-art scientific algorithms;
- Stratospheric vertical columns, by comparing with correlative ground-based measurements from the NDACC network (both in unpolluted and polluted conditions) and with other satellite data;
- Tropospheric vertical columns, by direct comparison with other satellite data and with MAXDOAS measurements.

Figure 2 shows an illustration of the method, as published in Valks et al., 2011. Time series of monthly mean NO_2 columns measured from January 2007 until July 2010 within 300 km of OHP by the GOME (GDP 4.1), SCIAMACHY (TEMIS) and GOME-2 (GDP 4.5) instruments are compared. The plot is divided in 3 vertical panels, presenting respectively the slant, stratospheric and tropospheric vertical columns. Similar seasonal variations are found between GOME-2 and the other datasets in all cases. The corresponding scatter plots are also included, with information about the results of a regression analysis of GOME-2 with respect to the other datasets. The correlation coefficients R are generally higher than 0.9 (except for the tropospheric columns) and the slopes S are generally close to one.

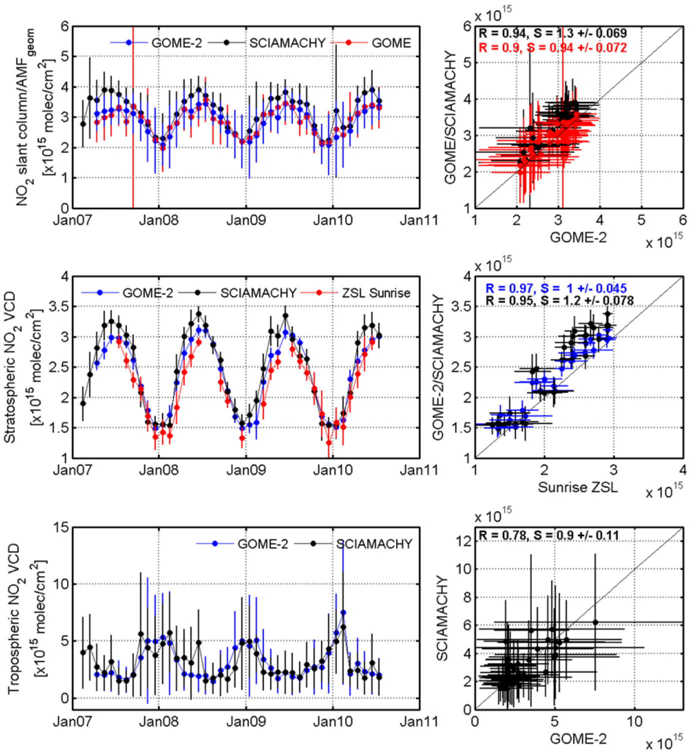

Figure 2: **Comparison of the time series of NO_2 slant, stratospheric and tropospheric columns measured by GOME (GDP 4.1), SCIAMACHY (TEMIS) and GOME-2 (GDP 4.5) between January 2007 and July 2010. The dots represent the monthly means of all the pixels within a radius of 300km around OHP and the error bars represent the variability (one sigma standard deviations). Adapted from Valks et al. 2011.**

2.2 Independent comparison with NDACC ground-based instruments

Comparison of the total/stratospheric NO_2 column of GOME-2 with UV-vis zenith-sky instruments from the NDACC network has been implemented during CDOP-1, including eventual corrections for stations affected by tropospheric pollution (Pinardi et al., 2011). In figure 3, two examples are presented, with comparisons above OHP and above Kerguelen (49°S, 70°E). As can be seen, above OHP a very stable behaviour of GOME-2 is obtained, while above Kerguelen a systematic and yet unexplained bias is found, with GOME-2 columns ~0.7×10^{15} molec/cm² lower than the ground-based data. Over time, the quality remains constant and no new issues, a part the systematic under-estimation of GOME-2 NO_2 at mid-latitudes in SH, have been identified.

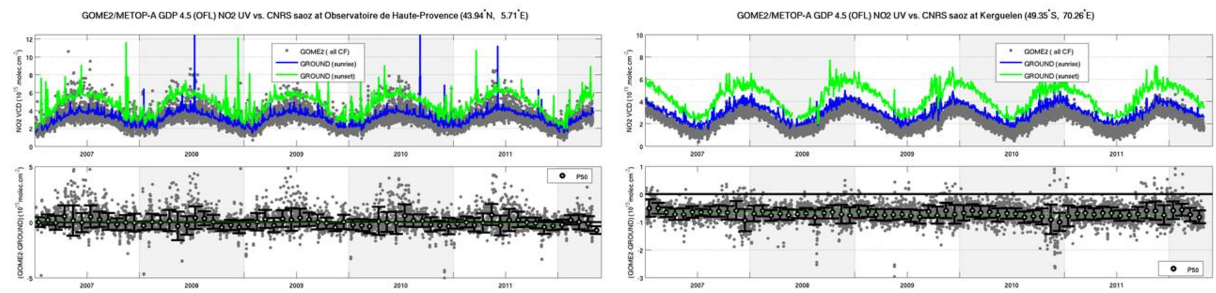

Figure 3: **Comparison of the time series of NO_2 total column of GOME-2 GDP 4.5 and the ground-based sunrise and sunset SAOZ data, between January 2007 and April 2012. In the lower subplots the light grey dots present the GOME-2 minus ground-based sunrise data and the black dots are the monthly means and standard deviation of the differences.**

2.3 Independent comparison with BIRA ground-based MAXDOASes

Comparison of the tropospheric NO_2 column of GOME-2 with BIRA-IASB MAXDOAS data from OHP and Beijing stations has been started during CDOP-1 (Pinardi et al., 2011). The MAXDOAS station of Uccle (Belgium) has been added since May 2011, and the MAXDOAS in Beijing centre has been moved to the Xianghe station, in its neighbourhood (~60km south-east of Beijing) since March 2011. As can be seen in Figure 4, with these three stations, very different conditions of tropospheric NO_2 are sampled, from clean/remote region (OHP), city (Uccle) and then heavily polluted region inside and outside Beijing. Good correlations between GOME-2 and the ground-based MAXDOAS data are obtained, both in terms of correlation coefficients R and slopes of the regression analysis S, for the three locations.

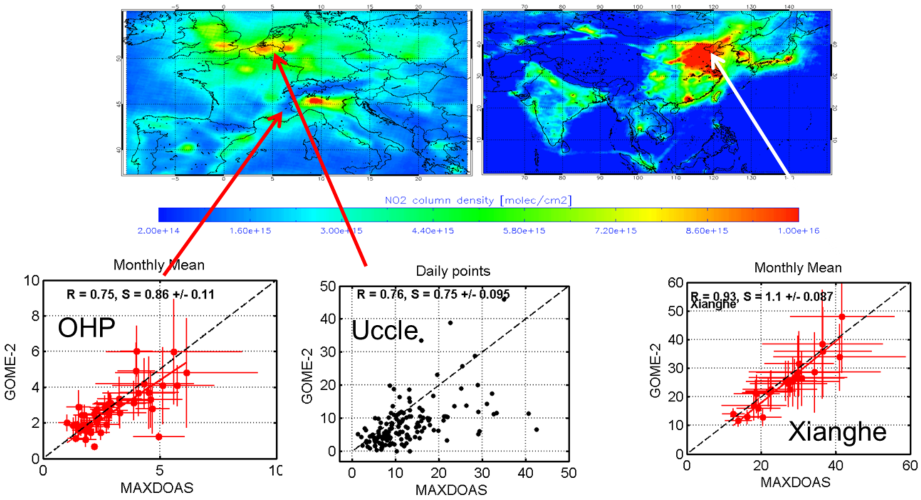

Figure 4: **Maps of tropospheric NO_2 from GOME-2 and the location of the BIRA MAXDOAS stations. The correlation plots corresponding to time-series presented in Figure 5 are given for each station in the lower panels. Either monthly means or daily points are showed.**

For the comparison with GOME-2, ground-based data are extracted within a time window of ±1h around the satellites overpass time and only cloud free pixels (CF<20%) within 100 or 50km are used (clean or polluted regions). Figure 5 presents the time-series of GOME-2 and ground-based MAXDOAS tropospheric NO_2 data both in terms of daily points and monthly mean comparisons. OHP is an interesting site for the study of low levels of tropospheric NO_2, as it alternates between clean air conditions and situations where it is influenced by polluted air masses transported from source regions. The Chinese case is very interesting as the measurements have been performed in two location, in Beijing city centre, on top of IAP building (40°N, 116.3°E) from June 2008 to April 2009, and then slightly outside the city (~60km south-east), showing very different results. In the first part of the measurement, the MAXDOAS data are much higher than GOME-2, while in Xianghe the difference between the two instruments is smaller. The Uccle location is characterized by intermediate pollution conditions.

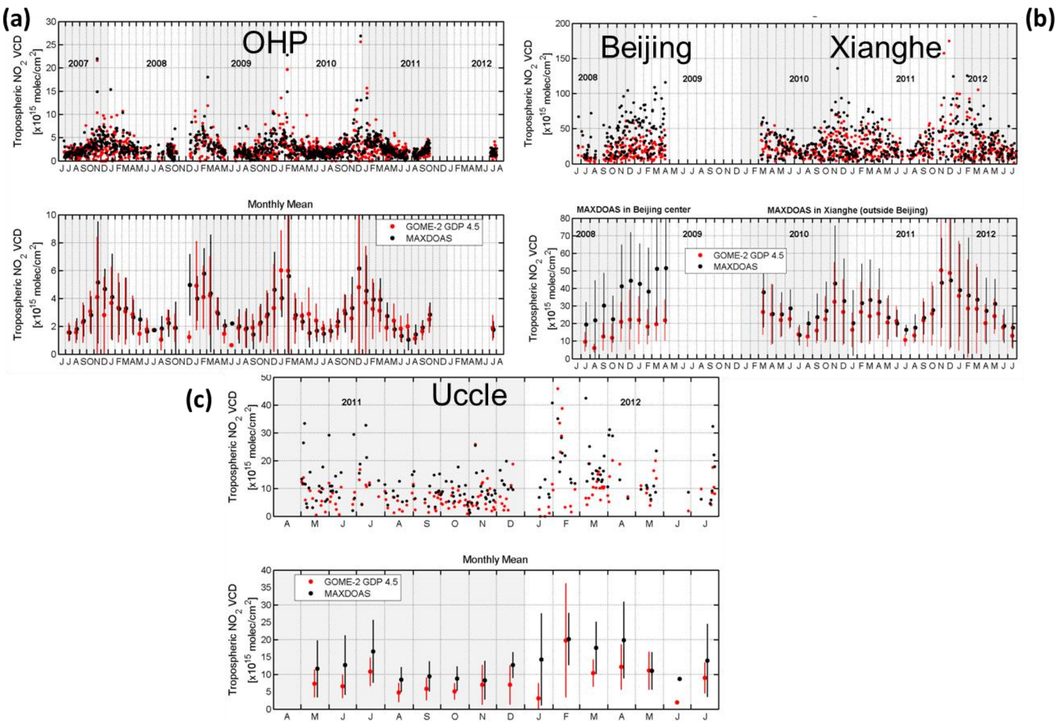

Figure 5: **Time series of MAXDOAS and GOME-2 GDP4.5 tropospheric NO_2 VCD above (a) OHP (since July 2007), (b) Beijing/Xianghe (in June 2008-April 2009 and since April 2010) and (c) Uccle (since May 2011). For each station, the daily points and the monthly mean values are given.**

Generally, one can see that pollution episodes are well captured by GOME-2 at the 3 locations and the comparisons of monthly averaged columns show consistent seasonal variations, with high NO_2 in winter and low NO_2 in summer. Very good agreement of the tropospheric NO_2 is obtained, except when the MAXDOAS is located in the city, where the measurements are more sensitive to local pollution peaks, while these tend to be smeared out in the satellite pixel. Part of the differences might also be related to uncertainties in the applied satellite retrieval settings (such as the choices of the a-priori NO_2 profiles, the cloud treatment, …). A study on the impact of the choice of the NO_2 a-priori profile is on-going for the Chinese locations.

3. VALIDATION ACTIVITIES: BRO

The validation of total BrO columns of GOME-2 was also a task of CDOP-1 and the first report (Theys et al., 2009) showed GOME-2 and SCIAMACHY total BrO columns agreed fairly well, although GOME-2 data exhibits a slightly different seasonal pattern than SCIAMACHY and generally lower values at high latitudes in both hemispheres. Since then, the scientific BrO product has been improved (Theys et al., 2011), by making use of a different wavelength analysis window. An example of the impact on one day of measurements with GOME-2 is shown in Figure 6. These new settings are currently under implementation in the operational system.

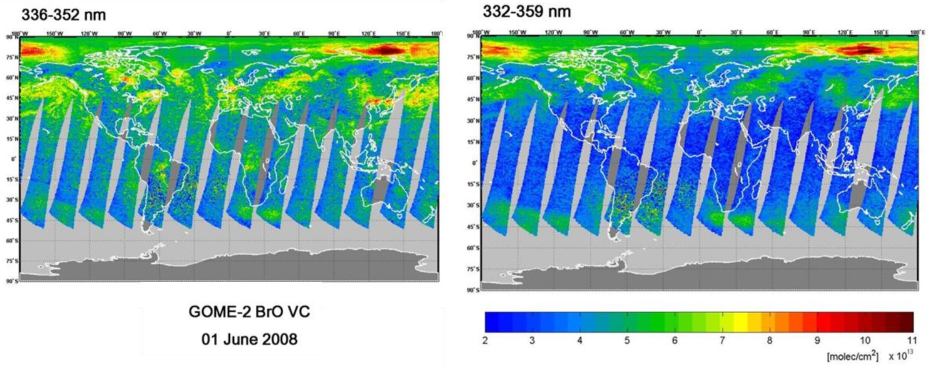

Figure 6: Effect of the change in fitting window on the total BrO columns **for the 1rst June 2008, taken from Theys et al. (2011).**

The validation of the improved total BrO columns has been performed over the period 2007-2010, both by comparisons with SCIAMACHY (Figure 7) and by comparisons with ground-based total BrO columns obtained at Harestua and Lauder (Figure 8). Both exercises show good agreement between GOME-2 and correlative data, as for the seasonal and latitudinal dependencies. Note that the differences are within the target accuracies defined for the BrO product (Fig. 7b) (Hovila et al., 2011).

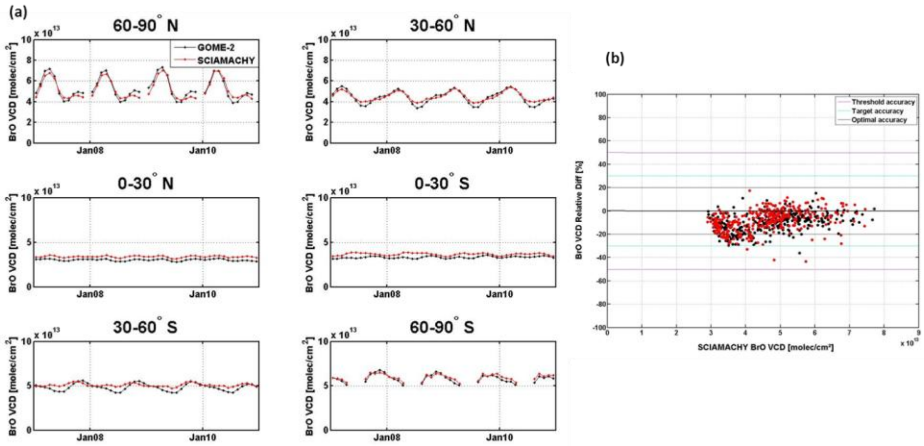

Figure 7: **(a) Comparison of the time series of BrO vertical column data measured by GOME-2 (black) and SCIAMACHY (red) between January 2007 and November 2010 for several latitudinal bands. (b) Differences between GOME-2 and SCIAMACHY, as a function of the SCIAMACHY BrO column and comparison to the threshold, target and optimal accuracy levels.**

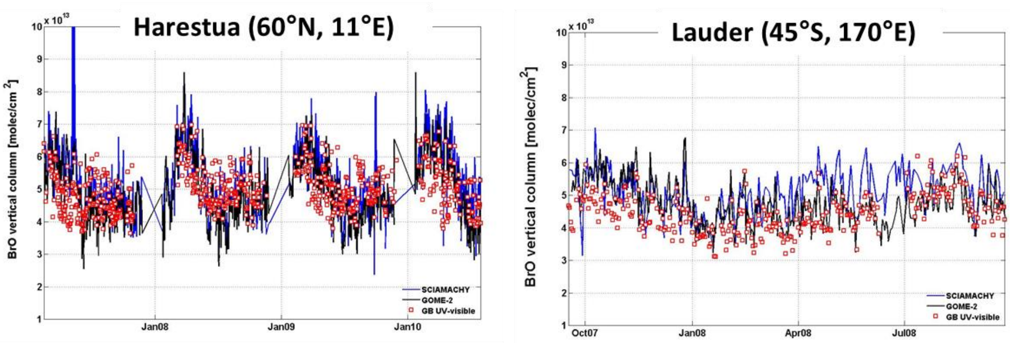

Figure 8: **Comparison of the time series of BrO vertical column data measured by GOME-2 (black), SCIAMACHY (blue) and ground-based zenith-sky data (red) at Harestua and Lauder, over the period 2007-2010.**

4. VALIDATION ACTIVITIES: H_2CO

The validation of H_2CO columns of GOME-2 was also included in CDOP-1 and the first report (De Smedt et al., 2010) showed that most of the differences between the scientific and operational products were due to different auxiliary databases, such as the albedo and the clouds. Recently, the H_2CO scientific GOME-2 product have been ameliorated (De Smedt et al., 2012), improving the coherence with SCIAMACHY and reducing the impact of the GOME-2 degradation effects. Figure 9 shows e.g., the H_2CO slant column standard deviation over the Equatorial Pacific from GOME, SCIAMACHY and GOME-2, scaled to a pixel size of 10x10km^2. It can be seen that compared to GOME-2 v07 (the operational product version), version v12 (the improved scientific product settings) have reduced standard deviations (~20% in 2007) and that the GOME-2 degradation has a smaller effect on H_2CO columns. These improved settings will be implemented in the operational product during CDOP-2.

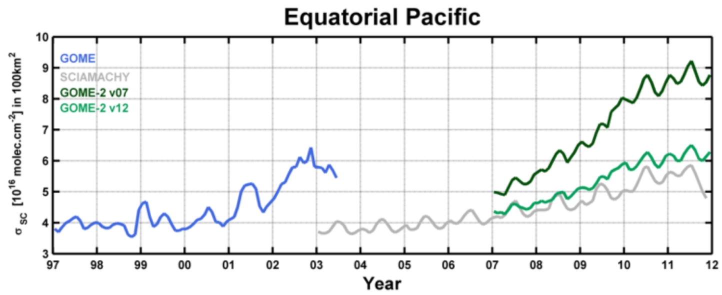

Figure 9: **Comparison of the time series of H_2CO slant column standard deviation over the Equatorial Pacific from GOME, SCIAMACHY and GOME-2, scaled to a pixel size of 10x10km2. GOME-2 v07 is the version with the DOAS settings implemented in the operational product (as in De Smedt et al., 2008) while version v12 is the new scientific product with improved DOAS settings as in De Smedt et al., 2012.**

Validation of the improved v12 GOME-2 scientific data has been started, including comparisons to SCIAMACHY data and to ground-based measurements in La Reunion and in China (Figures 10 and 11).

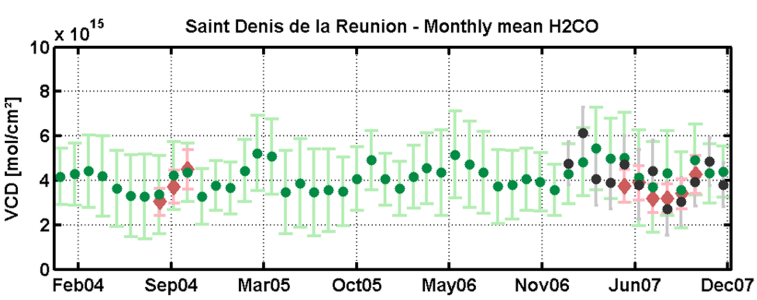

Figure 10: **Comparison of the time series between monthly averaged GOME-2 (black) and SCIAMACHY (green) H_2CO columns over the time period 2004-2007, with results from two FTIR campaigns at La Reunion (red dots).**

Figure 10 shows a comparison between monthly averaged GOME-2 and SCIAMACHY H_2CO columns with results from two FTIR campaigns held at La Reunion in 2004 and 2007. In addition, figure 11 displays a comparison between monthly averaged GOME-2 and SCIAMACHY H_2CO columns with MAX-DOAS and Direct-Sun measurements in Beijing and Xianghe from 2008 until early 2012. The

GOME-2 data are presented with two different choices of H_2CO a-priori profile: the IMAGES profile (used all over the globe in the GOME-2 operational algorithm and for SCIAMACHY) and an H_2CO profile obtained from the MAXDOAS data using the profiling method described in Clemer et al., 2010. It can be seen that GOME-2 agrees very well to SCIAMACHY data in the first case, and that the satellite data are smaller than the ground-based MAXDOAS and Direct-Sun data. When using the MAXDOAS profile as a-priori for the GOME-2 retrieval, a much better agreement with the ground-based data is obtained, pointing systematic differences near the surface between the modelled and the ground-based measured profiles.

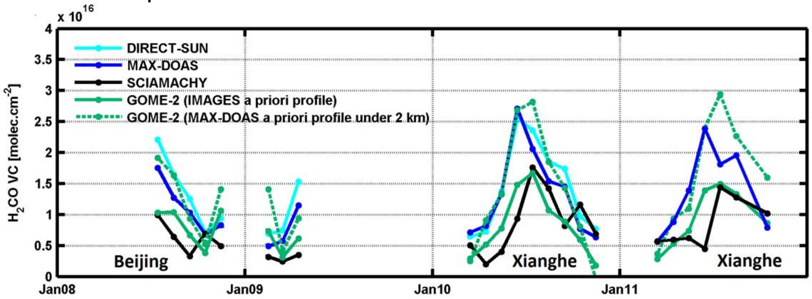

Figure 11: **Comparison of the time series from June 2008 to now, between monthly averaged GOME-2 (green), SCIAMACHY (black) and ground-based MAXDOAS (dark blue) and Direct-sun (light blue) H_2CO columns over Beijing and Xianghe.**

For the verification and quality assessment, an end-to-end approach of comparison of the operational product with the scientific product is in development, by studying the different components of the H_2CO algorithm, such as the slant columns (SCD), the air mass factors (AMF), the vertical columns (VCD), as well as some external dataset information, such as the cloud fractions (CF). An example over South Asia is shown in Figure 12. In addition to this verification, a quality assessment with external data was planned, based on SCIAMACHY and OMI data. However, since the loss of Envisat in March 2012 and the fast degradation of the OMI H_2CO columns over the period 2005-2011, a monthly climatology based on the GOME-2 scientific product over selected regions (Figure 13) will be used as baseline for the quality assessment in the web portal.

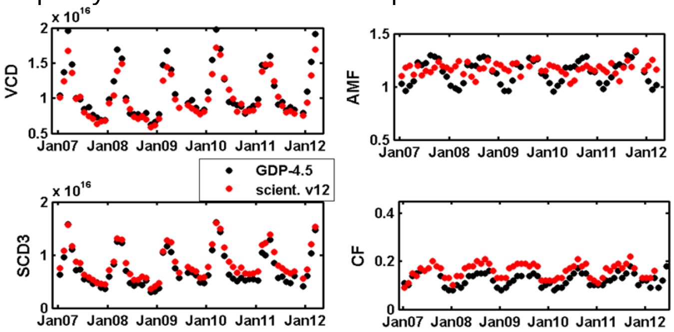

Figure 12: **Example of the end-to-end comparison of the time series of H_2CO columns between the operational GDP-4.5 and the scientific v12 product over the South Asian region (Lat: [12°, 22°] and Long: [98.5°, 110°]).**

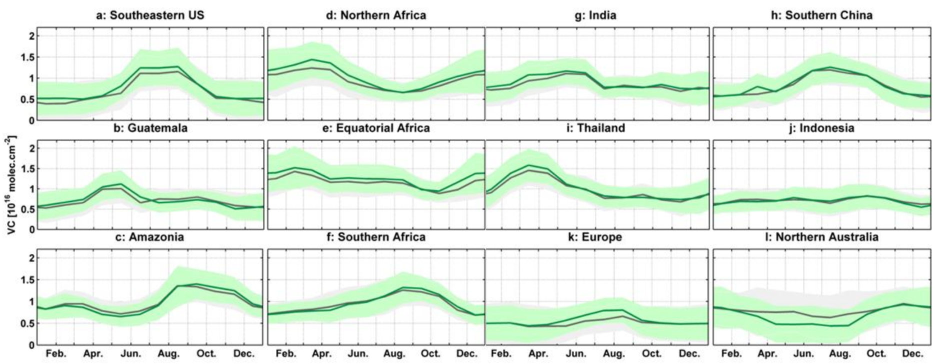

Figure 13: Monthly climatology based on the GOME-2 (in green) scientific product over an ensemble of selected regions. The corresponding SCIAMACHY monthly climatology (in grey) is shown for comparison.

4. CONCLUSIONS AND FUTURE WORK

Based on the heritage and experience from CDOP-1, BIRA-IASB is coordinating the GOME-2 minor trace gases validation and quality assessment for the O3M-SAF. Several gases are already continuously validated (NO_2, BrO, H_2CO,…) and latest results have been shown here. Validation of other gases, such as SO_2 are currently extended (comparison of GOME-2 and IASI SO_2 data over volcanoes) and in the next years, the expansion to other trace gases measured by GOME-2 and IASI (such as glyoxal, HNO3 and OClO) is planned, including both Metop-A and on Metop-B.
The results will be regularly updated and presented on a validation and QA web portal that is under development at BIRA-IASB. This trace gas validation system will largely benefit from harmonization and automatization of the ground-based remote-sensing data within the NORS project.

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