

ENVISAT / SCIAMACHY VALIDATION WITH THE LPMA / DOAS / MINI-DOAS BALLOON GONDOLA: COMPARISON OF O₃, NO₂ AND BRO PROFILES

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ABSTRACT

Level 2 products (profiles of O₃, NO₂, BrO) of the Envisat/SCIAMACHY instrument are validated by balloon-borne measurements of the same quantities using the same optical technique. The comparison studies with the level 2 retrievals of the University of Bremen are encouraging. Generally, the satellite and the balloon-borne O₃ retrievals agree within 15 to 20 % above 15 km. For NO₂, a good agreement within about 20% is observed down to 18 km. At lower altitudes the relative differences increase, reaching about 40% at 15 km. For BrO we revisit the study of [1] which validates the scientific BrO product. A good agreement within about 20% is found between 15 and 25 km for measurements at mid and high-latitudes. The comparison for a tropical balloon flight shows, however, larger discrepancies of about 20-50%.

1. INTRODUCTION

The SCanning Imaging Absorption spectroMeter for Atmospheric CHartography (SCIAMACHY) instrument onboard the European Environmental Satellite (Envisat) is an UV/visible/near-IR spectrometer designed to measure direct and scattered sunlight in various viewing directions [2].

Here, we briefly report on the efforts made to validate SCIAMACHY level 2 products by balloon-borne solar occultation UV/visible spectroscopy (DOAS instrument) and limb scattered skylight measurements (mini-DOAS instrument). So far, the LPMA/DOAS payload (Limb Profile Monitor of the Atmosphere / Differential Optical Absorption Spectroscopy) has been deployed on 5 validation campaigns conducted at high, mid and low-latitudes (Tab. 1). For all flights, the

payload was equipped with a UV/visible DOAS spectrometer [3], a Fourier transform spectrometer [4] and a mini-DOAS instrument [5]. Best matches of correlative measurements with the SCIAMACHY satellite instrument were identified using an air mass trajectory matching technique (section 2.2). For photochemically sensitive gases a suitable correction scheme is employed, in order to correct for illumination (daytime) mismatches in the individual measurements. For more details of the employed methods, techniques and scientific results see e.g. [1], [5], [6] and [7].

2. METHOD

The validation studies comprise the following methods and tools.

2.1. Instrumentation and trace gas retrieval:

The French/German LPMA/DOAS balloon payload comprises three optical spectrometers, which analyze direct sunlight over virtually the entire wavelength range from the UV to the mid-IR and thus essentially cover the same wavelength range as SCIAMACHY. Since 2002, additionally, a small versatile UV/visible spectrometer (referred to as 'mini-DOAS') is routinely deployed on the same gondola and observes scattered skylight in limb scattering geometry (like SCIAMACHY) [5]. It offers the advantage in recording the diurnal variation of profiles of the targeted gases, which allows a temporal match with respective satellite measurements. Details of the setup and operational performance of the instruments are described, e.g., in [4], [3] and [5]. Thus only a short description of the instrumental features important for SCIAMACHY validation is given here. The LPMA/DOAS

Table 1: Compendium of LPMA/DOAS observations and coincident Envisat / SCIAMACHY overpasses. BA and SO indicate balloon ascent and solar occultation measurements, respectively.

Balloon flight date, time/UT	Location	Geophysical condition	Available datasets	Satellite coincidence orbit, date, time/UT	Altitude range/km	Time delay/h	Spatial distance/km
04 Mar. 2003 13:20–16:17	Kiruna 67.9°N, 21.1°E	High-lat. spring SZA: 71.1°–94.1°	SO: LPMA	5273, 4 Mar., 11:05 5285, 5 Mar., 7:17	20–30 23–24	–5.1 +15.3	369–496 498–499
23 Mar. 2003 14:47–17:28	Kiruna 67.9°N, 21.1°E	High-lat. spring SZA: 78.9°–94.7°	BA: LPMA, DOAS SO: LPMA, DOAS	5545, 23 Mar., 11:07 5558, 24 Mar., 9:01 5545, 23 Mar., 11:07 5558, 24 Mar., 9:01	18–28 19–29 20–30 17–30	–5.2 +17.4 –6.2 +16.0	268–496 10–495 63–458 256–453
9 Oct. 2003 15:39–17:09	Aire sur l'Adour 43.7°N, 0.3°W	Mid-lat. fall SZA: 72.0°–87.8°	BA: DOAS	8407, 9 Oct., 9:51 8421, 10 Oct., 9:20	17–31 25–33	–6.5 +17.2	738–988 547–977
24 Mar. 2004 14:04–17:31	Kiruna 67.9°N, 21.1°E	High-lat. spring SZA: 74.5°–95.3°	BA: DOAS SO: DOAS	10798, 24 Mar., 10:35 10812, 25 Mar., 10:04 10798, 24 Mar., 10:35 10812, 25 Mar., 10:04	12–33 6–16 10–33 10–20	–5.4 +19.9 –6.9 +16.7	371–499 32–485 191–436 301–475
17 June 2005 18:32–21:13	Teresina 5.1°S, 42.9°W	Tropical winter SZA: 60.6°–95.8°	BA: DOAS SO: DOAS	17240, 17 June, 11:53 17255, 18 June, 13:02 17240, 17 June, 11:53 17255, 18 June, 13:02	25–30 5–33 23–32 8–33	–8.1 +18.4 –9.1 +16.2	382–491 6–490 519–971 12–496
27 June 2008 05:22–21:18	Teresina 5.1°S, 42.9°W	Tropical winter SZA: 60.4°–95.7°	SO: DOAS	33058, 26 June, 13:04 33072, 27 June, 12:32 33072, 27 June, 12:34	18–30 12–35 12–38	–19.9 +3.9 +3.9	416–989 540–991 160–543

spectrometers are deployed on an azimuth-controlled gondola operated by CNES (Centre Nationale d'Etudes Spatiales). The optical setup, including an automated sun-tracker, guarantees that the UV/visible (DOAS) and IR (LPMA) spectrometers analyze direct light. Solar occultation measurements are performed during balloon ascent or descent and during sun-rise and sun-set with moderate spectral resolution in the UV/visible (UV: FWHM = 0.5 nm, visible: FWHM = 1.5 nm) and high spectral resolution in the IR (unapodized resolution 0.02 cm⁻¹).

From the direct sunlight spectra, slant column amounts of the targeted atmospheric absorbers are inferred, using the DOAS approach in the UV/visible [8]. Upon trace gas retrieval the measured slant column amounts or absorptions of the measured species are inverted into trace gas profiles by applying the truncated Singular Value Decomposition (SVD) or the Maximum A Posteriori (MAP) inversion technique [9]. For the profile inversion of reactive species (e.g. NO₂ and BrO), a correction based on photochemical modelling is included [6].

The mini-DOAS is deployed on different azimuth-controlled balloon platforms (LPMA/DOAS, MIPAS-B2, LPMA/IASI) where it detects limb scattered skylight from different tangent heights by scanning actively through the atmosphere. The recorded spectra are analyzed using the same technique as for the direct sun spectra (DOAS) to infer slant column amounts of O₃, NO₂, BrO and HONO (and possibly in future also of OClO, IO, OIO and CH₂O) [5]. Additionally radiative transfer modelling is required to (a) simulate the measured quantities and recheck the input to the model and (b) to infer vertical profiles of the measured trace gases. From subsequent scans through the atmosphere, we can infer time series of trace gas profiles, which provide a dedicated tool for a direct match to satellite measurements.

2.2. Trajectory modelling:

Balloon-borne measurements are inherently restricted by different constraints, limiting their flexibility in satellite validation. Air mass trajectory modelling is used in order to find the best coincidences between air masses probed by the balloon-borne instruments and the satellite instrument.

The trajectory model uses the operational analyses and forecasts of the European Centre for Medium Range Weather Forecasts (ECMWF) - or a combination of both - given every 6 h on a 2.5° x 2.5° latitude/longitude grid. The ECMWF data are interpolated to 25 user-defined isentropic levels extending from the surface up to 1600 K. The internal time step for integrating the path of the air masses is 10 min and the diabatic and climatological heating rates are based on Newtonian cooling. The results (trajectory points) are stored for each hour (e.g. [10], [11]).

Backward and forward trajectories are started at the balloon measurement locations, which depend on the individual measurement technique and observation geometry. For the LPMA / DOAS remote-sensing payload, the start and end points are calculated from knowledge of the balloon flight trajectory and the known observation geometry given by the line-of-sight for each measurement. For post-flight analysis, forward and backward trajectories are calculated for up to 10 days, but for balloon flight planning purposes the time range is limited by the available ECMWF forecasts.

The actual geolocations of SCIAMACHY observations are taken from the SCIAMACHY Operational Support Team (SOST) on their website (<http://atmos.af.op.dlr.de/projects/scops>). Here, the overpass time, the geolocation and detailed measurement specifications (e.g. swath, measurement duration, ground-pixel size) are downloaded for the SCIAMACHY limb and for the SCIAMACHY nadir mode for each Envisat orbit. For the air mass trajectory-based matching technique only the area covered by

tangent points (light blue areas in Fig. 1) of SCIAMACHY limb observation is considered in the analysis in more detail. This information is used to find satellite measurement points along individual air mass trajectories, for which the spatial and temporal mismatch is as small as possible. The match criterion is chosen based on the experience of the ozone Match experiment e.g. [11], [12]: a time mismatch between the satellite observation and the air mass trajectory started at the balloon observation of $< \pm 1$ h and an area mismatch of $< \pm 500$ km. If SCIAMACHY observations do not fulfill these criteria, the distance criterion is extended up to 1000 km.

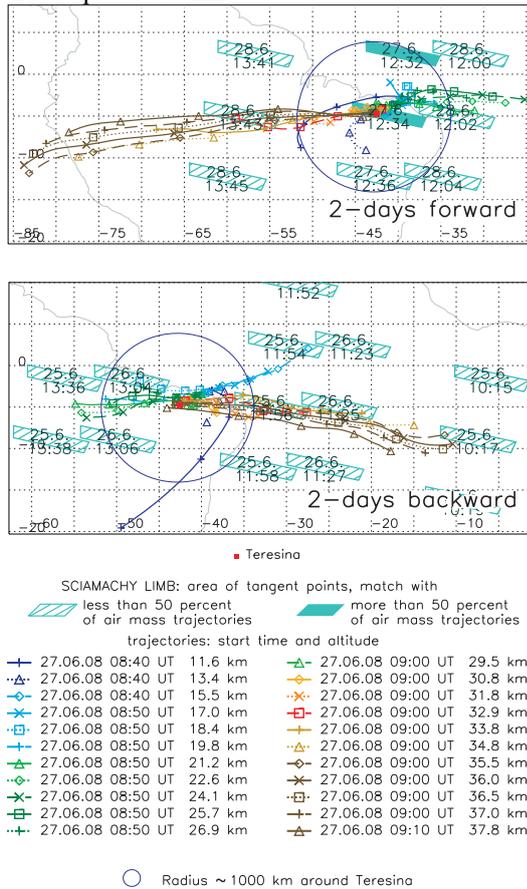


Figure 1. Air mass trajectories modelled 48 hours forward (upper panel) and backward (lower panel) in time for the balloon sunrise measurements of the LPMA/DOAS payload at Teresina on June 27, 2008. The trajectories are color-coded according to their starting altitude as indicated in the legend. A symbol is plotted every 12 hour interval. The areas covered by the tangent points of SCIAMACHY limb observations are projected onto the Earth's surface and illustrated as blue rectangles. Filled/shaded rectangles correspond to SCIAMACHY limb observations for which more/less than 50% of the calculated air masses are coincident with the balloon measurements. The time and date are indicated [11].

2.3. Photochemical modelling:

A 1-D column model is used to reconstruct the diurnal cycle for comparison with the observations. The vertical 1-D column model simulates stratospheric photochemistry on forward and backward air mass trajectories (described above) with the aim to find best guess profiles for the satellite observations based on the different validation balloon measurements. The stratospheric photochemistry is modelled on 20 potential temperature (Θ) levels between $\Theta = 323$ K and $\Theta = 1520$ K. The 1-D column model is initialized, at each height level, at 00:00 UT with 3-D CTM SLIMCAT [13] model results at an adjacent 48 hour model time step at the balloon launch site.

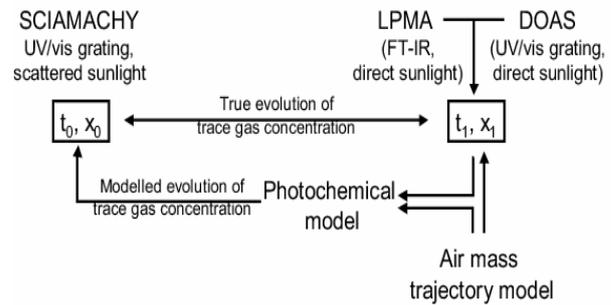


Figure 2. Schematics of the presented validation strategy. SCIAMACHY observations are conducted at time t_0 and location x_0 . Prior to the balloon flight dedicated to SCIAMACHY validation, an air mass trajectory model is used to optimize the time t_1 and location x_1 of the LPMA / DOAS balloon-borne observations, e.g. by optimizing the launch time of the balloon. After the balloon flight, the trajectory model calculates the air mass history in order to identify satellite measurements, which actually sampled the same air masses as the balloon-borne instruments. For the validation of photochemically active trace species, the illumination history of the coincident air masses is fed into a photochemical model to reproduce the evolution of the considered trace gases between satellite and balloon-borne observations as realistically as possible and to infer appropriate scaling factors. Figure adopted from [6].

The model is constrained to follow the evolution of the SZA time-line, which is taken from the air mass trajectory calculations. In satellite validation, these measures guarantee that the photochemical evolution of the modelled air mass is a good approximation of the true evolution between initialization of the model, the satellite measurement and balloon-borne observation. For simplicity a single representative SZA time-line is chosen for all Θ levels and the model is run with fixed pressure and temperature for each Θ level taken from the meteorological support data of the balloon flight.

Furthermore, each observation conducted by the remote sensing instruments SCIAMACHY and LPMA/DOAS is a composite of changing photochemical conditions (due to changing SZA) along the line-of-sight. Photochemical-weighting factors are calculated to scale balloon observations to the photochemical conditions of the satellite measurements. In the case of LPMA / DOAS measurements the scaling is implicitly considered by the profile inversion algorithm as described by [6]. A flow diagram of the overall validation procedure is given in Fig. 2.

3. PRODUCTS & RESULTS

Validation of level 2 products:

We report on 6 LPMA / DOAS validation balloon flights performed since 2003. Three balloon flights were conducted from ESRANGE, Kiruna, Sweden, one from Aire sur l'Adour in southern France and two from Teresina, northeastern Brazil (see Tab. 1). For each balloon flight a satellite coincident measurement is identified in the morning before and after the balloon flight using the trajectory matching technique described above (Fig.1). In the following we refer to these coincidences as backward and forward coincidences. If trace gas profiles inferred from balloon ascent and solar occultation are available, the satellite coincidences are identified separately. For each balloon flight Tab. 1 provides information on the measurement site, the geophysical condition, the SZA range covered by the balloon-borne observations, the available data sets and some details on the selected SCIAMACHY limb scans.

3.1. NO₂ and O₃ validation:

Fig. 3 shows an illustrative comparison between SCIAMACHY NO₂ profiles inferred by the IUP-Bremen retrievals (version 3.1) and the coinciding LPMA / DOAS balloon-borne observations. The relative deviations between the satellite and all available balloon-borne observations are shown in Fig. 4 (update of Figure 9 in [6]). In the 20 km to 30 km altitude range the agreement between the balloon-borne NO₂ profiles and the satellite observations is on the order of $\pm 20\%$ and most often well represented by the combined error bars. Down to 15 km, the relative differences between SCIAMACHY and balloon-borne measurements increase with decreasing altitude to about 40% with SCIAMACHY results generally being lower than the balloon-borne data. Below 15 km the agreement gets worse with the relative differences exceeding 50% which is most probably due to a decreasing sensitivity of the SCIAMACHY retrievals at these altitudes. Thus for low altitudes the SCIAMACHY retrieval might depend on the actual parameters, e.g. a priori information. The latter finding is supported by the characteristics of the corresponding averaging kernels (not shown).

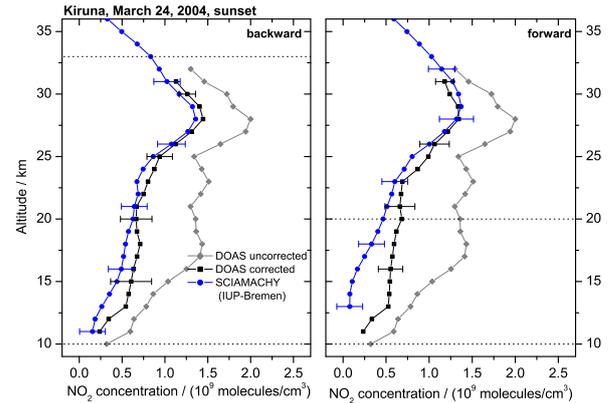


Figure 3. Comparison of NO₂ profiles inferred from SCIAMACHY limb observations with correlative balloon-borne measurements. The observations were conducted at Kiruna on March 24, 2004, during sunset. The left and right panel corresponds to a backward and a forward coincidence, respectively. Satellite data inferred by IUP-Bremen are shown as blue circles. Appropriately smoothed DOAS data are plotted as black boxes. The grey diamonds represent DOAS profiles at full altitude resolution. The altitude range between the horizontal dotted lines represents the range where coincident air masses are found. For better visibility, only selected error bars are shown.

Comparisons of O₃ profiles retrieved from the SCIAMACHY limb measurements at IUP Bremen (version 2.2) show a good agreement within the entire altitude range. Generally, relative differences between the two data sets are on the order of 15-20%. However, below 15 km, some outliers with too low O₃ concentrations resulting from SCIAMACHY retrievals are observed.

Deviations in the lower layers might be due to the lower sensitivity of the satellite retrieval or unaccounted horizontal trace gas variations.

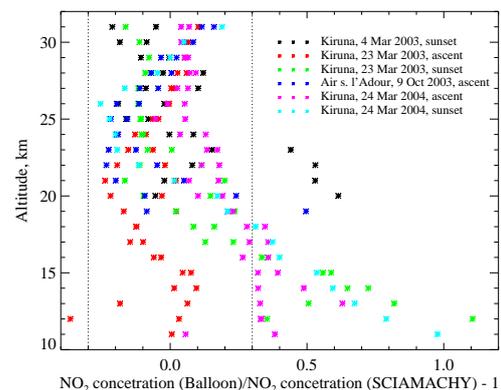


Figure 4. Relative deviations between SCIAMACHY (IUP-Bremen) and LPMA / DOAS measurements of NO₂. Filled and open symbols correspond to backward and forward coincidences, respectively.

3.2. BrO validation:

The BrO profiles retrieved at mid and high-latitudes from SCIAMACHY limb measurements agree mostly within 20% with co-located photochemically [1] corrected balloon-borne observations (Kiruna and Air sur l'Adour launches). The agreement is best between 15 and 25 km. Above 25 km the relative differences are slightly higher reaching about 30% which is most probably due to lower signal to noise ratio of the SCIAMACHY limb spectra at higher tangent heights – see Fig.5. Below 15 km the sensitivity of SCIAMACHY retrievals decreases resulting in a higher relative differences with respect to collocated balloon-borne measurement of up to 50%. For a tropical profile (only one profile in the comparison) originating from the Teresina balloon flight on 17 June 2005, the agreement is worse as compared to other flights with the relative deviation varying from 10 to 60% between 17 and 30 km. In this altitude range the SCIAMACHY profiles for both forward and backward match are lower as compared to the collocating balloon-borne observation. Below 17 km the statistical error of both SCIAMACHY and balloon-borne profiles is too high making the comparison results less meaningful.

The University of Bremen currently coordinates a comparison study for the algorithms and retrieval results from IUP-Bremen, MPI-Mainz, DLR and Harvard-Smithsonian (BOOST project – Alexei Rozanov).

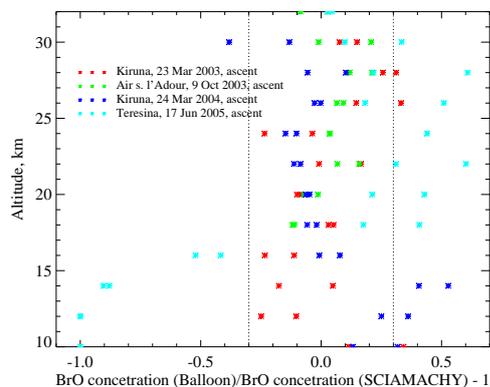


Figure 5. Same as Fig. 4, but for BrO.

3.3. Validation with the mini-DOAS instrument:

An advantage of balloon-borne scattered skylight measurements as compared to direct sun measurements in satellite validation results from the potential to record the diurnal variation of the targeted species, rendering photochemical modelling unnecessary (see Fig. 6). For the example shown in Fig. 6 recorded during an LPMA/IASI balloon flight at Teresina, northeastern Brazil on June 30 2005, a collocated NO₂ profiling with SCIAMACHY was possible (white line at 14 UT, at SZA = 34°) at a distance of 570 km. It is found that overall both NO₂ profiles excellently agree in particular

above 26 km (Fig. 7), which provides further confidence of the employed methods.

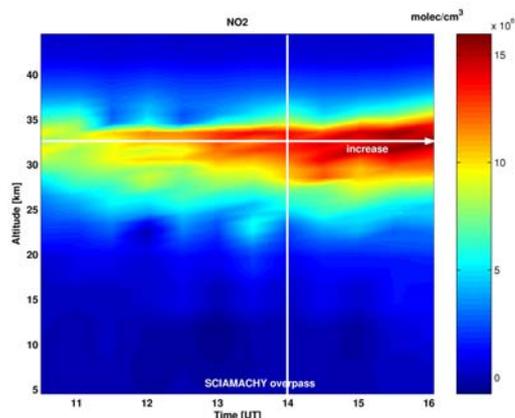


Figure 6. Diurnal variation of NO₂ measured by balloon-borne limb scattered skylight observation at Teresina, Brazil on June 30, 2005.

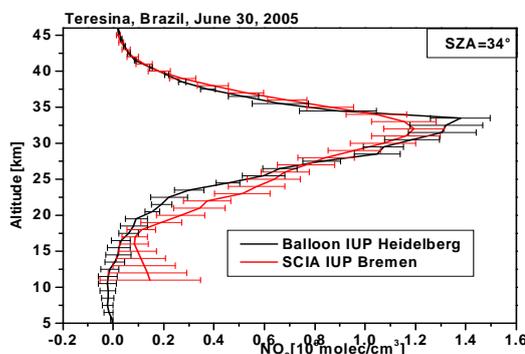


Figure 7. Concentration of NO₂ retrieved from SCIAMACHY measurements in orbit 17427-32 by IUP Bremen (red) and from balloon-borne measurements, retrieved by IUP Heidelberg (black), both at SZA=34° on June 30, 2005.

4. SUMMARY & CONCLUSION

Results from the 6 LPMA/DOAS and 13 mini-DOAS validation flights:

- Variable good agreement is obtained for level 2 products (BrO, NO₂ and O₃)
- In general comparisons indicate an accuracy of: ± (20 - 30) % for NO₂ and BrO (except for tropical measurements), and ± (15 - 20)% for O₃.
- A BrO comparison study is coordinated by the University of Bremen for the algorithms and retrieval results from IUP-Bremen, MPI-Mainz, DLR and Harvard-Smithsonian (BOOST project – Alexei Rozanov)
- Air mass trajectory calculations prove to be an important and powerful tool in satellite validation e.g. for coinciding balloon flights and satellite

overpasses planning and for the calculation of the photochemical change of the targeted species.

- Mini-DOAS observations are very purposeful for satellite validation, due to reasonable large degrees of information content (~10 vs. few for the satellite obs.) and the potential to monitor the time dependency of radicals, thus rendering photochemical corrections for collocated observations unnecessary.
- Upcoming validation activities will include an LPMA/DOAS and mini-DOAS flight from Kiruna in summer 2009.

The methods presented here are discussed in detail in [1], [5] and [6]. They are also of value for the validation of other existing satellite measurements of BrO, NO₂ and O₃ (e.g. GOME-2, OMI).

For future validation studies including operational products from ESA, digital copies of all balloon-borne DOAS related products for all validation flights, can be obtained from the NILU data server (<http://www.nilu.no>), upon signing the data protocol of the ESA sponsored Envisat validation activities.

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