



Milestone report covering MS 12

Milestone date: 30/06/2013

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Introduction

The milestone of the 30th of June 2013 (M20) concerns:

- MS 12 Guidelines for re-analysis of timeseries

A two months delay had been requested and accepted for this milestone.

MS 12 Guidelines for re-analysis of timeseries

The purpose of this milestone is to achieve a harmonized data analysis for NORS re-analysed products. In the following the guidelines for each technique are listed:

I. LIDAR:

Spectral region:

307.9 -308.2 nm (emitted wavelength) and
331.7 -332.1 nm (Raman channel)

Temperature profile used:

At OHP:

Daily P and T from local sounding (0 - 25 km) + NCEP (26-45) + MAP 85 (45-60 km)

At La Reunion: Daily P and T from local sounding (0 - 25 km) + Arletty model (25 -60 km)

Cross section used :

At OHP, Bass and Paur (1984)

At La Reunion, Brion, Daumont and Malicet (BDM, 1995)

Following the ASCO meeting ("Absorption Cross Sections of Ozone") in June 2013, the lidar O₃ CNRS team are waiting for a new O₃ cross section data set from Bremen institute. Depending of the new cross section, the lidar team will choose between this new cross section and BDM.

A new way of the vertical resolution calculation and a new definition of the resolution (impulse response) might be added in our data processing programme depending on the recommendation from the ISSI Lidar Team in September 2013.

II. MWR:

Re-analysis procedure and quality control of MW data in RDDS

The ozone profiles of MW are delivered to RDDS within four weeks. Before consolidation of the ozone data in the NDACC data center, the retrieved time series of ozone profiles should be checked and manually controlled by the operator. In rare cases, ozone profiles of poor quality may come through the retrieval chain and into the RDDS. Such runaway data can be easily detected if the time series of a longer time interval, e.g., one year are checked by the operator.

The strategy of the re-analysis is

1) Collection of the ozone data of MW in RDDS for a time interval of about one year (RDDS data) before the consolidation is done.

2) Quality control before delivery of the MW data to the consolidated data directory of NDACC:

a) Outlier removal: Remove possible outliers in the ozone series (the operator can mark such profiles with a cursor on the screen, and a flag will be set for invalid ozone profiles in the database. It might be just 3-5 profiles per year. However it is always good to look at the ozone series - in addition to automatical threshold controls.)

b) Intercomparisons: Perform intercomparisons of the RDDS data and independent satellite data. This gives an estimate of the shape of the MW radiometer and retrieval. Uni Bern has an automatical visualization of the actual ozone series of GROMOS, Aura/MLS, and ECMWF on internet (only accessible for Uni Bern).

Present situation for MW at RDDS:

GROMOS at Bern has two versions in RDDS:

Version 4 for the old filter bench data FB (November 1994 - September 2011)

Version 5 for the new FFTS data (July 2009 - now)

Plans at Bern:

- Intercomparisons have been performed by Simone Studer (publication comes soon, Studer et al., 2013). These intercomparisons showed that version 5 has a high quality, and version 4 can be easily adjusted to version 5 (possibly by adding a constant which is well defined because of the measurement overlap of FB and FFTS)
- Submission of version 5 and the adjusted version 4 to the consolidated data directory at NDACC

Present situation at Ny-Ålesund:

- The data are uploaded to RDDS on a daily basis as soon as the auxiliary data, e.g. pressure and temperature model data are available. This is about 3-4 days after the measurement.
- Intercomparison to satellite data has been performed by Palm et. al. (2010).

Plans at Ny-Ålesund:

- The submission of the data from 2006 to 2009 is under progress and will be completed by the end of August 2013.
- The RDDS data from September 2012 to April 2013 will be replaced by consolidated data by the end of August 2013.

Further consolidation will be performed in a yearly interval, or quicker if a problem with the RDDS data becomes evident earlier.

References:

Palm, M.; Hoffmann, C. G.; Golchert, S. H. W. & Notholt, J.: The ground-based MW radiometer OZORAM on Spitsbergen -- description and status of stratospheric and mesospheric O₃-measurements Atmos. Meas. Tech., 2010, 3, 1533 – 1545.

Studer, S., K. Hocke, M. Pastel, S. Godin-Beekmann, N. Kämpfer: Intercomparison of stratospheric ozone profiles for the assessment of the upgraded GROMOS radiometer at Bern, submitted to ACPD, 2013.

III. FTIR:

O₃:

For ozone a common NDACC scheme is used [Vigouroux et al., 2008] as summarized below:

Spectral region:

MW: 1000 - 1005 cm⁻¹,

Additional optional MWs [cm⁻¹]:

782.56 - 782.86

788.85 - 789.37

993.30 - 933.80

Interfering species: H₂O, CO₂, CH₄, O₆68, O₆86

WACCM climatology

HITRAN 2008

Profile retrieval

CO:

Also for CO a common NDACC retrieval scheme [Angelbratt et al., 2011] is used:

Spectral region:

MWs [cm⁻¹] with interfering species:

2057.0 - 2058.0 O₃, CO₂, OCS

2069.56 - 2069.76 O₃, CO₂, OCS

2157.5 - 2159.15 O₃, CO₂, OCS, N₂O, H₂O

WACCM climatology

HITRAN 2008

Profile retrieval

CH₄:

For CH₄ an improved data analysis scheme has been proposed by Frank Hase. It has been tested with spectra from several sites: Izaña, Jungfraujoch, Karlsruhe and Kiruna [Sepúlveda et al., 2013]. By including sites of miscellaneous latitudes and observing altitudes different humidity conditions have been covered in this study.

Spectral region:

Microwindows [cm⁻¹]:

To improve the sensitivity (DOFs ~2.3) more MWs have been included:

2611.600, 2613.350 - aux HDO

2613.700, 2615.400

2835.550, 2835.800

2903.820, 2903.925

2914.700, 2915.150

2941.510, 2942.220 - aux H₂O, deweighting of subregion (2941.88, 2942.08)

Two of these MWs are auxiliary MWs to get the H₂O + HDO right. The CH₄ target windows suffer from low interference by other gases (CO₂, NO₂, HDO, H₂O). It is important to avoid propagation of CH₄ signals from the aux MWs into the target CH₄ solution, so use zeroing of the CH₄ Jacobean sections in the aux MWs.

A linelist was sent around to the NORS partners. It is largely identical to HIT08, only for the (extended) MWs selected so far line parameters have been adjusted. This linelist is a preliminary result of the DFG project on spectroscopy lead by M. Palm, Bremen. D. Dubrovica and F. Hase applied some adjustments, according to a preliminary analysis of cell measurements done by DLR (M. Birk, J. Loos, et al). The linelist allows us to achieve better fits, unfortunately the vertical slope of the tropospheric profile is probably a bit too steep. For all other species, HIT08 (including the HIT09 corrections for H₂O) are used, in the spirit of earlier decisions taken within the NDACC.

References:

Angelbratt, J., J. Mellqvist, D. Simpson, J. E. Jonson, T. Blumenstock, T. Borsdorff, P. Duchatelet, F. Forster, F. Hase, E. Mahieu, M. De Mazière, J. Notholt, A. K. Petersen, U. Raffalski, C. Servais, R. Sussman, T. Warneke, and C. Vigouroux: Carbon monoxide (CO) and ethane (C₂H₆) trends from ground-based solar FTIR measurements at six European stations, comparison and sensitivity analysis with the EMEP model, *Atmos. Chem. Phys.*, 11, 9253-9269, doi:10.5194/acp-11-9253-2011, 2011.

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Vigouroux, C., M. De Mazière, P. Demoulin, C. Servais, F. Hase, T. Blumenstock, I. Kramer, M. Schneider, J. Mellqvist, A. Strandberg, V. Velazco, J. Notholt, R. Sussmann, W. Stremme, A. Rockmann, T. Gardiner, M. Coleman, and P. Woods: Evaluation of tropospheric and stratospheric ozone trends over Western Europe from ground-based FTIR network observations, *ACP*, Vol. 8, 6865-6886, SRef-ID: 1680-7324/acp/2008-8-6865, 2008.

IV. UV-VIS

1. Introduction

All UV-Vis data products developed and used in NORS are based on the differential optical absorption spectroscopy (DOAS) method, which is based on a separation between a spectral inversion step giving integrated slant column amounts, and a subsequent conversion step which ultimately provides the end products (total, tropospheric or stratospheric columns, and/or vertical profiles of concentration). We first describe recommendations for slant column retrievals using DOAS, and then formulate recommendations to total column and profile retrieval steps.

2. Recommendations for slant column retrieval

The recommended settings for the DOAS retrieval of O₃, NO₂ and HCHO have been developed as part of the activities of the NDACC UV-Vis working group and as a result of the CINDI intercomparison campaign (Peters et al., 2012). They are summarized in Tables 1 to 3.

	RECOMMENDED SETTINGS	COMMENTS
Fitting interval	450-550 nm	This range covers three bands of O ₃ differential absorption in the Chappuis region while minimizing contamination by water vapor and O ₄ absorption bands.
Wavelength calibration method	Calibration based on reference solar atlas	The Chance and Kurucz (2010) solar atlas is recommended as wavelength registration reference
Cross-sections		
O₃	Bogumil et al, (2003), 223° K	O ₃ absorption cross-sections measured with the SCIAMACHY flight-model instrument. The temperature dependence of the ozone absorption is weak in the Chappuis bands and can be neglected.
NO₂	Vandaele et al. (1998), 220° K	This reference is the one included in the HITRAN data base.
H₂O	HITRAN (2009)	The use of updated and recent versions of the HITRAN data base is recommended
O₄	Hermans et al. (2003)	
Ring effect correction method	NDACC source spectrum for Ring effect correction	It is recommended to use of an effective Ring cross-section. A high resolution Ring effect cross-section source (generated after Chance and Spurr, 1997) is provided on the NDACC web site.
Polynomial term	Polynomial of order 3 to 5 maximum	
Intensity offset correction	Slope	The intensity offset parameter corrects for spectral stray-light effects and for the wavelength dependence of the probability of Raman scattering (Ring effect). One usually recommends a slope correction (linear).

Table 1: Recommendations for the O₃ slant column spectral fit.

	RECOMMENDED SETTINGS	COMMENTS
Fitting interval	425-490 nm	Settings adequate for simultaneous NO ₂ and O ₄ retrieval with MAXDOAS instruments. For UV instruments, the alternative 400-450 nm interval is recommended. SAOZ instruments not stabilised in temperature are using the larger 433-530 nm interval in order to reduce interferences with strong solar lines and to gain

		in precision in the iterative analysis process.
Wavelength calibration method	Calibration based on reference solar atlas	The Chance and Kurucz (2010) solar atlas is recommended as wavelength registration reference
Cross-sections		
NO₂	Vandaele et al. (1998), 220° K	This reference is the one included in the HITRAN data base. For stratospheric NO ₂ columns, fine adjustment of temperature effects can eventually be performed in a post-processing step using a simple monthly zonal climatology of temperature profiles. For tropospheric NO ₂ columns, the temperature dependence of the NO ₂ cross sections should be taken into account, at least by selecting cross sections at the appropriate temperature or by adding a second (pseudo) cross sections set.
O₃	Bogumil et al, (2003), 223° K	O ₃ absorption cross-sections measured with the SCIAMACHY flight-model instrument.
H₂O	Harder and Brault (1997)	
O₄	Hermans et al. (2003)	
Ring effect correction method	Chance and Spurr (1997)	It is recommended to use of an effective Ring cross-section. A high resolution Ring effect cross-section source (generated after Chance and Spurr, 1997) is provided on the NDACC web site. Note that this approach neglects the impact of the Ring effect on the NO ₂ absorption itself (molecular Ring effect), which leads to a systematic underestimation of the NO ₂ slant columns by about 5%.
Polynomial term	Polynomial of order 3 to 5 maximum	
Intensity offset correction	Slope	The intensity offset parameter corrects for spectral stray-light effects and for the wavelength dependence of the probability of Raman scattering (Ring effect). One usually recommends a slope correction (linear).
Data filtering for clouds	Enhancement of O ₄ and/or H ₂ O absorption	Clouds have a small effect on stratospheric NO ₂ . However, it is recommended to remove measurements showing large enhancements of O ₄ and/or H ₂ O slant columns.

 Table 2: Recommendations for the NO₂ slant column spectral fit.

	RECOMMENDED SETTINGS	COMMENTS
Fitting interval	336.5-359 nm	
Wavelength calibration method	Calibration based on reference solar atlas	The Chance and Kurucz (2010) solar atlas is recommended as wavelength registration reference
Cross-sections		
H₂CO	Meller and Moortgat (2000), 293K	Two sources of H ₂ CO cross sections exist in the literature: Cantrell et al. (1990) and Meller and Moortgat (2000). They differ by about 9%
O₃	Bogumil et al, (2003), 223 K I ₀ -corrected	Using the alternative data set of Brion, Daumont, and Malicet (BDM, Daumont et al., 1992; Malicet et al., 1995) gives H ₂ CO DSCDs larger by ~5 x 10 ¹⁵ molec/cm ² .
NO₂	Vandaele et al. (1998), 298 K I ₀ -corrected	Switching to the alternative data set of Burrows et al. (1998) has an impact of ~2-5% on H ₂ CO DSCDs
BrO	Fleischmann et al. (2004), 223 K	Switching to the alternative data set of Wilmouth et al. (1999) has an impact of ~2% on H ₂ CO DSCDs.
O₄	Greenblatt et al. (1990)	The wavelength corrected O ₄ Greenblatt et al. (1990) cross sections are recommended (Pinardi et al., 2013).

Ring correction method	effect	Chance and Spurr (1997)	Uncertainties on H ₂ CO DSCDs are expected to be linked to the strength of the Ring effect, which itself is a function of the geometry, SZA, and aerosol content. The typical uncertainties related to this effect is in the 5-12% range.
Polynomial term		Polynomial of order 5	
Intensity correction	offset	Slope	

Table 3: Recommendations for the H₂CO slant column spectral fit (based on Pinardi et al., 2012).

A data base of absorption cross section data sets is available at <http://www.ndacc.org/>.

3. Total O₃ and stratospheric NO₂ vertical columns

Total O₃ and stratospheric NO₂ vertical columns are derived from zenith-sky UV-vis observations at twilight using the following expression:

$$VCD(\theta) = \frac{DSCD(\theta) + RCD}{AMF(\theta)} \quad (1)$$

where $VCD(\theta)$ is the O₃ (NO₂) vertical column density at solar zenith angle (SZA) θ , $DSCD(\theta)$ is the O₃ (NO₂) differential slant column density at SZA θ (amount of O₃ (NO₂) present in the optical path that the light follows to the instrument minus that from a reference measurement), RCD is the residual ozone amount in the reference measurement (a fixed spectrum usually recorded at high sun around local noon), and $AMF(\theta)$ the airmass factor at SZA θ .

Given expression (1), the retrieval of vertical columns consists of four steps: (1) slant column spectral fitting, (2) determination of residual amount in the reference spectrum, (3) conversion of absolute slant columns into vertical columns using appropriate AMFs, and (4) averaging of the vertical columns over a limited SZA range around 90° SZA. For the sake of harmonizing the different data sets provided to the NDACC database, the NDACC UVVIS Working Group has formulated recommendations for the processing of total O₃ and NO₂ columns. These are available from the NDACC web site (<http://www.ndacc.org/>) and, for the ozone case, they are described in more details in Hendrick et al. (2011).

3.1 Determination of the residual amount in the reference spectrum

In case of O₃, it is recommended to use a fixed control spectrum, selected at high solar elevation under stable ozone conditions. The residual amount in this reference spectrum should be determined using the Langley plot method based on Vaughan et al. (1997). For NO₂, chemically modified Langley plots are the preferred approach to determine the residual NO₂ amount in the reference spectrum. Alternative more empirical approaches such as the minimization of the diurnal variation of the NO₂ vertical columns are also suitable. The Langley plot method should be used to filter data contaminated by tropospheric NO₂ (data points not lying on a “smooth” line indicate a tropospheric contamination).

3.2 AMFs for the conversion of slant columns into vertical columns

A climatology of O₃ AMFs based on the TOMS version 8 (TV8) ozone and temperature profile climatology (Barthia et al., 2004) has been generated by BIRA with the aim to homogenize and consolidate the time-series of total ozone measurements produced by UV-VIS and SAOZ spectrometers of the NDACC network. The AMF climatology consists of 18 look-up tables, each of them corresponding to one TOMS TV8 latitude (10° latitude bands between 90°S and 90°N). The other entry parameters are: wavelength, ground albedo, altitude of the station, day of the year, and SZA.

A similar approach has been adopted for NO₂. The NDACC NO₂ AMF climatology has been built by BIRA based on the harmonic climatology of stratospheric NO₂ profile developed by Lambert et al. (1999, 2000). This AMF climatology consists of 2 look-up tables (one for sunrise and one for sunset conditions) with the following entry parameters: latitude, day of the year, wavelength, ground albedo, altitude of the station, and SZA. The NO₂ photochemistry at twilight has not been taken into account in the standard AMF calculation since it is rather complex to implement at a global scale. The impact of this assumption on the twilight NO₂ VCDs is of about 5-10%.

Interpolation routines have been developed to extract O₃ and NO₂ AMFs for a given station. The AMF climatologies and corresponding extraction routines are available from the NDACC web site (<http://www.ndacc.org/>). It should be noted that these O₃ and NO₂ AMFs are only suitable for background aerosol conditions.

3.3 Averaging of vertical columns around 90° SZA

The best compromise between accuracy and precision is achieved by averaging O₃ and NO₂ vertical columns in the 86-91° SZA range. The recommended approach is to apply a linear fit on vertical columns in the above SZA range and then derive the column value at the effective SZA. The NORS/NDACC UVVIS Working Group is currently working at the estimation of the effective SZA corresponding to the averaged O₃ and NO₂ vertical columns. So far, it is recommended to use 90° SZA.

4 Tropospheric profiles of NO₂, H₂CO, and aerosols

Tropospheric profiles of NO₂, H₂CO, and aerosol extinction are retrieved by applying an inversion algorithm to NO₂, H₂CO, and O₄ DSCDs measured at the different elevation angles of each MAX-DOAS scan. These data products are new and still under development. Generally speaking, MAXDOAS trace gas retrievals proceed in two-steps. First, the aerosol extinction vertical profile is retrieved from O₄ DSCDs which is necessary to account for the effect of aerosol on the light path through the atmosphere. Second, appropriate block AMFs and corresponding weighting functions are calculated using the retrieved aerosol extinction profile and they are used to retrieve vertical profiles of the various target trace gases.

4.1 Recommended approaches for the vertical profile inversion

Two different approaches are used within NORS to retrieve vertical profiles of trace gas concentration and aerosol extinction from MAX-DOAS measurements: the Optimal Estimation Method (OEM; Rodgers 2000) that gives vertical distributions of aerosols and trace gases on a defined altitude grid (e.g., 0 to 4 km by 200m step) and a more simple parameterized retrieval scheme that gives a first order description of typical vertical distributions, namely height and shape of well mixed layers starting at the surface, with

possibly an additional elevated layer (e.g. Vlemmix et al., 2011; Wagner et al., 2011). In brief, in the OEM formalism, the profile inversion is performed using weighting functions that describe the relation between the measured DSCDs and the vertical profile of interest, a priori profiles to constraint the retrieval and reject unrealistic solutions, and a priori and measurement uncertainty covariance matrices. The weighting functions are calculated on-line using state-of-the-art radiative transfer models (RTMs). In the parameterization approach, look-up tables of trace gas SCDs and AMFs are generally calculated off-line for different sets of profile parameters values using a RTM and the forward model simulations are then fitted to the measured DSCDs using a least-squares minimization strategy.

Within NORS, the OEM formalism is used by BIRA-IASB, UBremen, INTA, and UH while MPIC follows the simple parameterization approach. Harmonization efforts are currently under progress (e.g. on the retrieval of cloud conditions), and at this stage in the project it is not possible to provide recommendations on the profile retrieval method and corresponding settings (e.g., altitude grid, a priori profile,...) for the re-analysis of MAX-DOAS measurements time-series.

5. References

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