Network for the Detection of Atmospheric Composition Change (NDACC)

UV-VIS Working Group

Recommendations for NO_2 column retrieval from NDACC zenith-sky UV-VIS spectrometers

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1. Introduction

One of the goals of the NDACC is to ensure that long term high quality data sets of a number of important atmospheric parameters are regularly delivered and made available to the scientific community. Protocols for data acquisition, data evaluation and quality assessment are defined as part of the activities of the different instrument working groups. Satellite validation studies have shown that the UV-Vis zenith-sky NO_2 column data sets currently submitted to the NDACC data base still suffer from residual inconsistencies due to (1) differences in the DOAS settings applied by the different data providers, in particular as regards the source and temperature of the NO_2 absorption cross-sections, and (2) a lack of homogeneity in the air mass factors applied to convert NO_2 slant columns into vertical columns. The aim of the present note and of its accompanying material is to provide the recommendations, tools and input data sets that are needed to improve the overall homogeneity of the UV-Vis (stratospheric) NO_2 column measurements. The guidelines described here are preliminary and open for discussion (see in particular section 5). The aim is to converge towards new NDACC standards for NO_2 column retrievals, to be applied for future measurements as well as for reprocessing of historical data sets.

2. DOAS retrieval settings

The following recommendations are based on experience from recent intercomparison exercises, in particular from The Cabauw Intercomparison campaign for Nitrogen Dioxide Measuring Instruments (CINDI) in 2009 (Roscoe et al., 2010; Piters et al., 2012).

	RECOMMENDED SETTINGS	COMMENTS
Fitting interval	425-490 nm	Settings adequate for simultaneous NO2 and O4 retrieval. The large water vapor absorption band at 510 nm is avoided.
Wavelength calibration method	Calibration based on reference solar atlas	For optimal DOAS retrievals, spectra should be aligned on an accurate atlas of solar lines. A good reference is Chance and Kurucz (2010).
Cross-sections		
NO_2	Vandaele et al. (1997), 220° K	The low temperature reference data set of Vandaele et al. (220° K) is adequate for stratospheric NO_2 retrievals. Fine adjustment of temperature effects can eventually be performed in a post-processing step.
O_3	Bogumil et al, (2003), 223° K	This data set (obtained from SCIAMACHY flight-model measurements) is characterized by an excellent signal/noise ratio in the Chappuis bands and a good consistency with values in the Huggins bands.
H_2O	Hitran	We recommend using the most recent updates of the HITRAN data base as a source. Alternatively the measured data set of Harder and Brault (1997) is also a good choice if limited to the the NO_2 spectral region.
O_4	Hermans et al. (2003)	Current O_4 absorption cross-section reference for the visible and near UV regions.
Ring effect correction method	Chance and Spurr (1997)	The Ring effect is due to inelastic Raman scattering by air molecules (N_2 and O_2). It is responsible for a smoothing effect that mostly affects the highly structured solar Fraunhofer lines. Ring effect is usually corrected as part of the DOAS fit using a pseudo cross-section. 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	Filters out the broadband atmospheric attenuation due to scattering by air and particles. High orders should be avoided to

		minimize the cross-correlation with molecular absorption differential structures.
Intensity offset correction	Slope	The intensity offset term corrects for possible additive biases in measured intensities, such as can be produced by spectral stray-light or incorrect dark-current correction. It also implicitly corrects for the wavelength dependence of the Raman scattering probability (not accounted for in the simple Ring correction outlined above).
AMF calculation	NDACC climatology of NO_2 AMFs	A generic climatology of NO_2 AMFs has been generated at IASB-BIRA for NDACC. This table is constructed using the harmonic climatology of stratospheric NO_2 profile of Lambert et al. (1999; 2000), complemented at low altitudes (below 17 km) by a climatology derived from SAOZ balloon soundings. It has been designed to be applicable at any NDACC station (see section 3 of this note). Note that the twilight photochemistry of NO_2 is not taken into account, which may introduce biases on the resulting vertical columns of about 5-10% (similar to the error introduced by the simplified Ring correction approach).
Determination of residual amount in reference spectrum	Modified Langley plot	If possible, modified Langley plots are the preferred approach to determine the residual NO_2 amount in the reference spectrum. Alternative more empirical approaches such as the minimization of the diurnal variation of the NO_2 VCD are also suitable.
SZA range used for twilight averaging of vertical columns	86° – 91° SZA	Best compromise between accuracy and precision is achieved in the 86-91° SZA range. The effective SZA of the reported NO_2 average should be explicitly mentioned in the data product.

3. NO_2 air mass factors climatology

As reported in the existing literature (e.g. *Sarkissian et al., 1995, Van Roozendael et al., 1994*), differences in the radiative transfer model, pressure and temperature profiles, NO_2 profile shape, and wavelength can have a significant impact (up to 10-15%) on the resulting NO_2 AMF values. For the sake of homogeneity, it is desirable to improve the level of standardization of the UV-Vis data evaluation process. We describe a new multi-entry data base of NO_2 AMFs applicable at the global scale.

The proposed data base of NO_2 AMFs is based on the harmonic climatology of stratospheric NO_2 profile developed by Lambert et al. (1999, 2000). This climatology consists of a Fourier harmonic decomposition of UARS HALOE v19 and SPOT-4 POAM-III v2 NO_2 profile data records. It has been used for the retrieval of global total ozone fields from recent European UV-VIS nadir sounders (GOME and SCIAMACHY). For the NO_2 AMF calculation, the NO_2 concentration between 20 and 60 km altitude is taken from the Lambert et al.'s climatology. Between 12 and 17 km, the NO_2 profiles are complemented by a climatology derived from SAOZ balloon observations (F. Goutail, personal communication). The NO_2 concentration is set to zero below 12 km altitude.

The parameters considered in building the NO_2 AMF climatology are: wavelength, ground albedo, altitude of the station, and SZA. Table 1 summarizes these different parameters and their corresponding values.

Parameter	**Values**
Lambert et al.'s NO_2 profile climatology	- Latitude: 85°S to 85°N step 10° - Month: 1 (Jan) to 12 (Dec) step 1

	- Sunrise and sunset - Altitude range : 20-60 km
SAOZ balloon NO_2 profile climatology	- Latitude: tropics, mid- and high-latitudes - Resolved in seasons (spring, summer, fall, winter) - Altitude range: 12-20 km
Wavelength	350 to 550 nm step 40 nm
Surface albedo	0 and 1
Altitude of the station	0 and 4 km
SZA	10, 30, 50, 70, 80, 82.5, 85, 86, 87, 88, 89, 90, 91, and 92°

Table 1: Parameters of the NO_2 AMF climatology and their corresponding values.

NO_2 AMFs have been calculated using the UVSPEC/DISORT radiative transfer (RT) model which includes a treatment of the multiple scattering in a pseudo-spherical geometry. This model has been validated through several intercomparison exercises (e.g. *Hendrick et al., 2006; Wagner et al., 2007*). An aerosol extinction profile corresponding to background conditions has been used for the AMF calculation. It has been constructed from the aerosol model of *Shettle* (1989) included in UVSPEC/DISORT, and is therefore not suitable for volcanic conditions. The O_3 and temperature profiles are from US Standard Atmosphere and the TOMS V8 climatology, respectively.

The NO_2 AMF climatology consists of 2 look-up tables (size: 416 KB each), one for sunrise and one for sunset conditions. An interpolation routine has been developed to extract appropriately parameterized NO_2 AMFs for the different NDACC stations. The interpolation routine is written in FORTRAN 77 and a DOS executable has been created. The source code is also available for compilation on LINUX machines. In addition, a global monthly climatology of the surface albedo at two wavelengths (380 and 494 nm) is coupled to the interpolation routine so that realistic albedo values can be obtained in a transparent way. This albedo climatology is extracted from the GOME surface albedo database developed by *Koelemeijer et al.* (2003). It consists of 24 (12x2) look-up tables, one for each month of the year and each wavelength. Albedo values are given for grid-cells of 1° x 1° (latitude: -89.5° to 89.5°; longitude: -179.5° to 179.5°).

4. How to use the AMF climatology?

The zip file contains 31 files: 2 NO_2 AMF look-up tables, 24 surface albedo look-up tables (size: 1.1 MB each), a DOS executable ('no2_amf_interpolation_dos'), the source code in FORTRAN 77 ('no2_amf_interpolation.for'), two input files for selecting parameter values, and 1 output file. All the files should be located in the same directory for a proper use of the climatology. In the file 'input_no2_amf.dat', the user can enter a value for wavelength, latitude, longitude, surface albedo, and altitude of the station. Regarding the albedo, the user has to give a value to a flag in order to determine whether he wants to use the albedo climatology (flag=1) or not (flag=2). The user has also to define the name of the file containing lines with year, decimal day numbers (decimals being decimal UT time), and SZAs at which AMF should be extracted (here this file is called 'DAY_SZA.dat'; maximum number of lines in this file: 500000). The last flag is for the display of the interpolation results on the screen (1: display; 2: no display). The resulting NO_2 AMFs are stored in a file called 'no2_amf_output.dat'.

5. Points for discussion

- Should we introduce a more refined (post-processing) correction for variations of the the stratospheric temperature (around 220°K)?

- How to filter data contaminated by tropospheric NO2?

- How to filter data for clouds – is it necessary?

- Should we explicitly correct for the impact of the Ring effect on the NO2 SCDs?

- Should we take into account the NO2 photochemistry and its impact on the AMF?

- How to derive best estimates of our random and systematic uncertainties? (both need to be reported according to GEOMS)

- For historical long data series going back to early 1990 or before: Is there a need to introduce an AMF correction for the period affected by the Pinatubo aerosols?

- More points??

6. References

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7. Contact

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