Network for the Detection of Atmospheric Composition Change (NDACC)

UV-VIS Working Group

Recommendations for total ozone retrieval from NDACC zenith-sky UV-VIS spectrometers

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1. Introduction

One of the key 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 working groups of the NDACC. Based on results presented and discussed at the last UV-Vis Working Group Meeting in November 2007, it was recognized that the UV-Vis total ozone 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 of the ozone absorption cross-sections, and (2) a lack of homogeneity in the air mass factors applied to convert O_3 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 homogeneity of the UV-Vis total ozone measurements delivered to the NDACC data base. It is anticipated that after eventual adjustments based on feedback provided by the WG members, the guidelines provided in this document will become NDACC standards for total ozone retrievals from UV-Vis instruments, to be applied for future measurements as well as for reprocessing of historical data sets.

2. Recommended settings for O_3 vertical column retrieval

The following recommendations have been jointly formulated during the November 2007 edition of the UV-VIS Working Group Meeting, held at BAS.

	RECOMMENDED SETTINGS	**COMMENTS**
Fitting interval	450-550 nm	This fitting range provides good sampling of the O_3 differential absorption structures, while avoiding contamination by the strongest water vapor and O_4 absorption bands.
Wavelength calibration method	Calibration based on reference solar atlas	We recommend that measured spectra be aligned according to Fraunhofer lines, on a atlas of solar lines such as Chance and Spurr (1997) or Kurucz (1984).
Cross-sections		
O_3	Bogumil et al, (2003), 223° K	These absorption cross-sections have been measured as part of the SCIAMACHY pre-flight calibration. They are characterized by an excellent signal/noise ratio in the Chappuis bands and good consistency with values in the Huggins bands.
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 and therefore adequate for NO_2 removal in the O_3 fitting range.
H_2O	Hitran 2004	Cross-sections generated using the latest version of the HITRAN data base should be used.
O_4	Greenblatt et al. (1990)	This data set is generally accepted as the baseline O_4 cross section reference. However care must be taken to use the wavelength scale corrected version of Burkholder. Note that a good alternative is the Hermans et al. data set (unpublished, available from www.aeronomie.be/spectrolab/o2.htm).
Ring effect correction method	NDACC source spectrum for Ring effect correction	For NDACC processing we recommend the use of an effective Ring cross-section to be included in the DOAS procedure. We provide a high resolution Ring effect cross-section source (generated after Chance and Spurr, 1997), to be convolved at appropriate instrumental resolution.
Polynomial term	Polynomial of order 3 to 5 maximum	The polynomial filters out the broadband atmospheric attenuation due to scattering by air and particles. It may also compensate for broadband structures due to changing instrumental response.

Intensity offset correction	Instrument dependent	The importance of this correction largely depends on the stray-light rejection capability of the spectrometer. At minimum, it is usually safe to allow for a flat offset correction.
AMF calculation	NDACC look-up table of O_3 AMFs	A generic look-up table of O_3 AMFs has been generated at IASB-BIRA for NDACC. This table is constructed using the TOMS version 8 column-resolved O_3 profile climatology. It has been designed to be applicable at any NDACC station (see section 3 of this note).
Determination of residual amount in reference spectrum	Langley plot	If possible (depending on long-term instrumental stability) we recommend the use of a fixed control spectrum, selected at high solar elevation under stable ozone conditions. The residual amount in this reference spectrum should be determined as recommended in Vaughan et al. (1997).
SZA range used for twilight averaging of vertical columns	86° – 90° SZA	Best compromise between accuracy and precision is achieved in the 86-90° SZA range. The effective SZA of the reported O_3 average should be explicitly mentionned in the data product.

3. A new LUT of O_3 AMFs based on the TOMS version 8 ozone profile climatology

A new climatology of O_3 AMFs has been generated with the aim to homogenize and consolidate the time-series of total ozone measurements produced by UV-VIS and SAOZ spectrometers from the NDACC. As reported in the existing literature (e.g. *Sarkissian et al., 1995, 1995b, Van Roozendael et al., 1998*), differences in the radiative transfer model, pressure and temperature profiles, ozone profile shape, and wavelength can have a significant impact (up to 5-10%) on the resulting O_3 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 O_3 AMFs applicable at the global scale. Its validity is tested through application at a few NDACC stations.

The proposed data base of O_3 AMFs is based on the TOMS version 8 (TV8) ozone and temperature profile climatology (*Barthia et al., 2004*). The TV8 is a monthly-zonal climatology sorted according to the ozone column. It has been widely used for the retrieval of global total ozone fields from recent US and European UV-VIS nadir sounders (e.g. *Barthia et al., 2004, Coldewey-Egbers et al., 2005, Van Roozendael et al., 2006, Eskes et al., 2005*).

The parameters considered in building the look-up table (LUT) are: wavelength, ground albedo, altitude of the station, and SZA. Table 1 summarizes these different parameters and their corresponding values.

Parameter	**Values**
TOMS v8.0 O_3 and temperature climatology	- Latitude: 85°S to 85°N step 10° - Month: 1 (Jan) to 12 (Dec) step 1 - Ozone: 125 to 575 DU step 50 DU (TOMS O_3 grid)
Wavelength	440 to 580 nm step 35 nm
Surface albedo	0 and 1
Altitude of the station	0 and 4 km
SZA	30, 50, 70, 80, 82.5, 85, 86, 87, 88, 89, 90, 91, and 92°

Table 1: Parameters of the look-up table and their corresponding values.

O_3 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. Therefore the present O_3 AMF climatology is not suitable for volcanic conditions.

The climatology consists of 18 look-up tables (size: 1.0 MB each), each of them corresponding to one TOMS latitude (table #1: 85°S…table #18: 85°N). An interpolation routine has been developed to extract appropriately parameterized O_3 AMFs for the different NDACC stations. Compared to version 1.0, the new version 2.0 of the routine allows AMFs to be interpolated on a yearly basis. The look-up tables are the same for both versions. 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 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 12 look-up tables, one for each month of the year. The wavelength corresponding to these tables is 494 nm and 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 34 files: 18 O_3 AMF look-up tables, 12 surface albedo look-up tables (size: 1.1 MB each), a DOS executable ('o3_amf_interpolation_v2_0_dos'), the source code in FORTRAN 77 ('o3_amf_interpolation_v2_0.for'), and two input files for selecting parameter values. All the files should be located in the same directory for a proper use of the climatology. In the file 'input_o3_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 with day numbers, SZAs and corresponding O_3 columns (here called 'Day_SZA_O3_col.dat'; maximum number of lines in this file: 500000) and to give a value to the flag for the interpolation on the O_3 column (fixed to 1 if the O_3 columns in 'Day_SZA_O3_col.dat' are vertical columns in DU and to 2 if O_3 columns are slant columns in molec/cm^2). The last flag is for the display of the interpolation results on the screen (1: display; 2: no display). The resulting O_3 AMFs are stored in a file called 'o3_amf_output.dat'.

5. Verification and examples of application to NDACC data

Previous studies have demonstrated that, for AMF calculation, the UVSPEC/DISORT model shows very good consistency with others RT models (see e.g. *Hendrick et al., 2006; Wagner et al., 2007*). Nevertheless, to firmly assess the reliability of the present calculations, a quick verification exercise has been undertaken in collaboration with Dmitry Ionov (St. Petersburg State University and CNRS/SA). AMF calculations based on identical settings were performed using both UVSPEC/DISORT and the SCIATRAN model from IUP-Bremen (see www.iup.uni-bremen.de/sciatran/index.html). These show that both RT models are in excellent agreement (difference less than 2 %) when initialized in the same way.

To qualitatively illustrate the impact of using the new O_3 AMF climatology in comparison to the often used standard mid-latitude value, time-series of AMFs have been calculated for one year of data at five stations of the SAOZ/NDACC network: Sodankyla (67.4°N, 26.6°E), Jungfraujoch (46.5°N, 8°E), Observatoire de Haute Provence (OHP; 43.9°N, 5.7°E), Bauru

(22.3°S, 46°W), and Dumont d'Urville (66.7°S, 140°E). These AMFs have been compared to standard AMFs calculated with temperature and O_3 profiles extracted from the US Standard Atmosphere. The wavelength was fixed to 541 nm, the albedo to 0, and the altitude to 0 km, except for Jungfraujoch (altitude: 3.58 km). Results are presented in Figure 1.

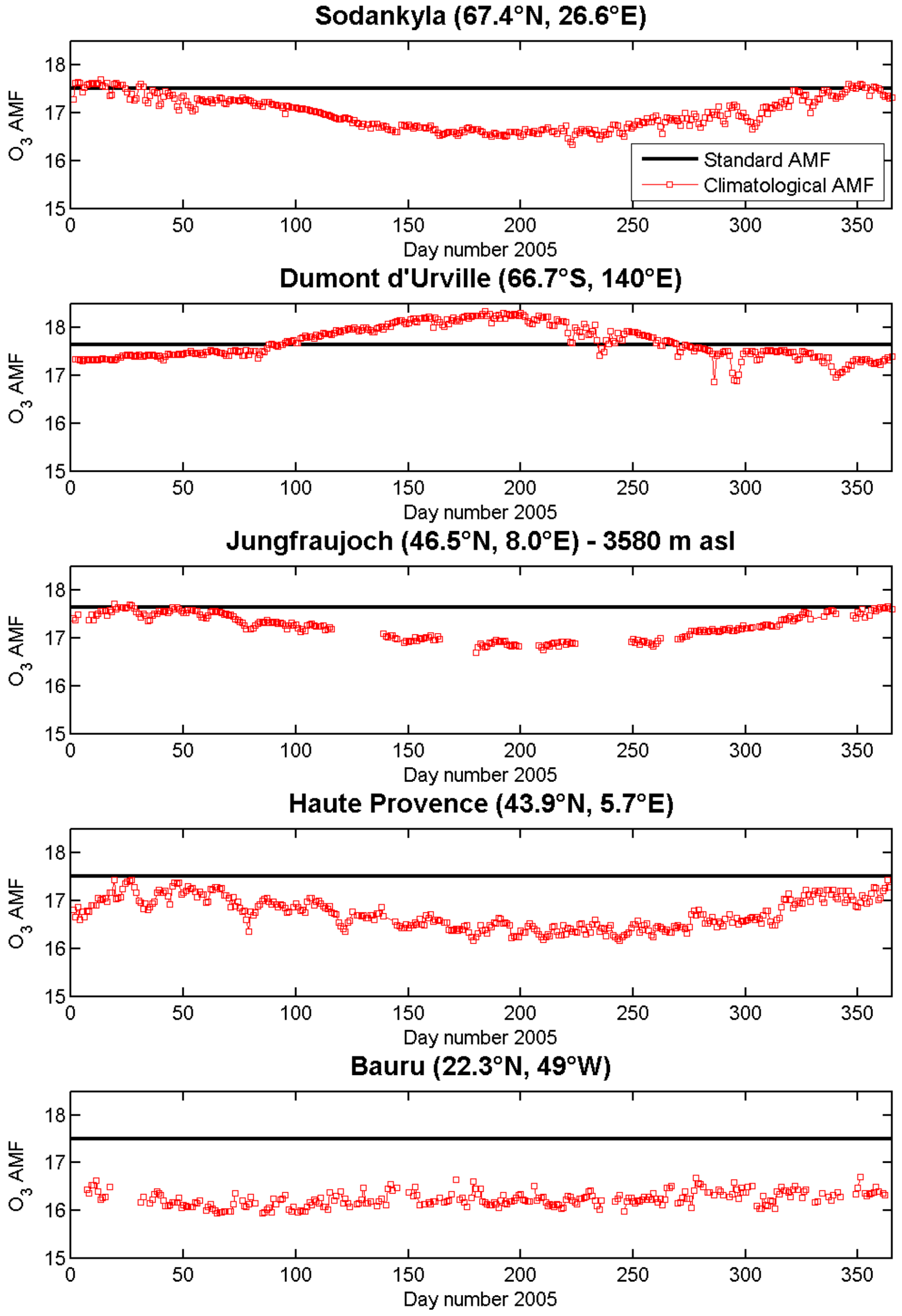

Figure 1: Comparison between climatological (red open squares) and standard (black line) O_3 AMFs at 90° SZA at Sodankyla, Dumont d'Urville, Junfraujoch, Observatoire de Haute Provence, and Bauru.

At mid- and high-latitude in the NH, the largest difference is obtained in summer with climatological AMFs smaller than the standard AMF by up to 8%. In winter, the difference is smaller than 2% at Sodankyla and Jungfraujoch but can reach 5%

at OHP (with still climatological AMFs smaller than standard ones). At high-latitude in the SH, the climatological AMFs are smaller than the standard AMFs in summer while the opposite feature is found in winter. The relative difference is smaller than 5%. In the tropics, the climatological AMFs are systematically smaller than the standard AMFs with relative difference in the 5-10% range.

6. References

Barthia, P. K., C. G. Wellemeyer, S. L. Taylor, N. Nath, and A. Gopolan, Solar Backscatter (SBUV) Version 8 profile algorithm, Proceedings of the Quadrennial Ozone Symposium 2004, edited by C. Zerefos, pp. 295-296, Athens, Greece, ISBN, 960-630-103-6, 2004.

Bogumil, K., J. Orphal, T. Homann, S. Voigt, P. Spietz, O.C. Fleischmann, A. Vogel, M. Hartmann, H. Bovensmann, J. Frerik, and J.P. Burrows, Measurements of molecular absorption spectra with the SCIAMACHY Pre-Flight Model: Instrument characterization and reference spectra for atmospheric remote sensing in the 230-2380 nm region, J. Photochem. Photobiol. A, 157, 167-184, 2003.

Burrows, J. P., A. Richter, A. Dehn, B. Deters, S. Himmelmann, S. Voigt, and J. Orphal, Atmospheric remote-sensing reference data from GOME: 2. Temperature-dependent absorption cross sections of O_3 in the 231-794 nm range, J. Quant. Spectrosc. Rad. Transfer, 61, 509-517, 1999.

Chance, K. and R.J.D. Spurr, Ring effect studies: Rayleigh scattering including molecular parameters for rotational Raman scattering, and the Fraunhofer spectrum, Applied Optics, 36, 5224-5230, 1997.

Coldewey-Egbers, M., M. Weber, L. N. Lamsal, R. de Beek, M. Buchwitz, and J. P. Burrows, Total ozone retrieval from GOME UV spectral data using the weighting function DOAS approach, *Atmos. Chem. Phys., 5*, 1015–1025, 2005.

Eskes, H. J., R. J. van der A, E. J. Brinksma, J. P. Veefkind, J. F. de Haan, and P. J. M. Valks, Retrieval and validation of ozone columns derived from measurements of SCIAMACHY on Envisat, Atmos. Chem. Phys. Discuss., 5, 4429–4475, 2005.

Greenblatt, G. D., J.J. Orlando, J.B. Burkholder, and A.R. Ravishankara, Absorption measurements of oxygen between 330 and 1140 nm, J. Geophys. Res., 95(D11), 18577-18582, doi:10.1029/90JD01375, 1990.

Hendrick, F., M. Van Roozendael, A. Kylling, A. Petritoli, S. Sanghavi, R. Schofield, C. von Friedeburg, F. Wittrock, and M. De Mazière, Intercomparison exercise between different radiative transfer models used for the interpretation of ground-based zenith-sky and multi-axis DOAS observations, Atm. Chem. Phys., 6, 93-108, 2006.

Koelemeijer, R. B. A., J. F. de Haan, and P. Stammes, A database of spectral surface reflectivity in the range 335-772 nm derived from 5.5 years of GOME observations, J. Geophys. Res., 108 (D2), doi 10.1029/2002JD002429, 2003

Kurucz, R.L., I. Furenlid, J. Brault, and L. Testerman, Solar flux atlas from 296 nm to 1300 nm, National Solar Observatory Atlas No. 1, 1984.

Sarkissian, A., H. K. Roscoe, D. Fish, M. Van Roozendael, M. Gil, A. Dahlback, L. Perliski, J.-P. Pommereau, and J. Lenoble, Ozone and NO_2 air-mass factors for zenith-sky spectrometers: intercomparison of calculations with different radiative transfer models, Geophys. Res. Lett., 22, 1113-1116, 1995.

Sarkissian, A., H. K. Roscoe, and D.J. Fish, Ozone measurements by zenith-sky spectrometers: an evaluation of errors in air-mass factors calculated by radiative transfer models, JQSRT, 54, 471-480, 1995b.

Shettle, E. P., Models of aerosols, clouds, and precipitation for atmospheric propagation studies, AGARD Conference Proceedings No. 454: Atmospheric propagation in the UV, visible, IR and mm-region and related system aspects, 1989.

Vandaele, A.-C., C. Hermans, P.C. Simon, M. Carleer, R. Colin, S. Fally, M.-F. Mérienne, A. Jenouvrier, and B. Coquart, Measurements of the NO2 absorption cross-section from 42000 cm-1 to

10000 cm-1 (238-1000 nm) at 220 K and 294 K, J. Quant. Spectrosc. Radiat. Transfer, 59, 171-184, 1998.

Van Roozendael, M., P. Peeters, H.K. Roscoe, H. De Backer, A.E. Jones, G. Vaughan, F. Goutail, J.-P. Pommereau, E. Kyro, C. Wahlstrom, G. Braathen, and P.C. Simon, Validation of Ground-Based Visible Measurements of Total Ozone by Comparison With Dobson and Brewer Spectrophotometers, J. Atm. Chem., 29, 55-83, 1998.

Van Roozendael, M., D. Loyola, R. Spurr, D. Balis, J-C. Lambert, Y. Livschitz, P. Valks, T. Ruppert, P. Kenter, C. Fayt and C. Zehner, Ten years of GOME/ERS-2 total ozone data—The new GOME data Processor (GDP) version 4: 1 Algorithm description, *J. Geophys. Res.* 111, D14311, doi:10.1029/2005JD006375, 2006.

Vaughan, G., H. K. Roscoe, L. M. Bartlett, F. M. O'Connor, A. Sarkissian, M. Van Roozendael, J.-C. Lambert, P. C. Simon, K. Karlsen, B. A. Kåstad Høiskar, D. J. Fish, R. L. Jones, R. Freshwater, J.-P. Pommereau, F. Goutail, S. B. Andersen, D. G. Drew, P. A. Hughes, D. Moore, J. Mellqvist, E. Hegels, T. Klupfel, F. Erle, K. Pfeilsticker, U. Platt, An Intercomparison of ground-based UV-visible sensors of ozone and NO_2, J. Geophys. Res., 102, 1411-1422, 1997.

Wagner, T., J. P. Burrows, T. Deutschmann, B. Dix, C. von Friedeburg, U. Friess, F. Hendrick, K.-P. Heue, H. irie, H. Iwabuchi, Y. Kanaya, J. Keller, C. A. Mc Linden, H. Oetjen, E. Palazzi, A. Petritoli, U. Platt, O. Postylyakov, J. Pukite, A. Richter, M. Van Roozendael, A. Rozanov, R. Sinreich, S. Sanghavi, and F. Wittrock, Comparison of box-air-mass-factors and radiances for multiple-axis differential optical absorption spectroscopy (MAX-DOAS) geometries calculated from different UV/visible radiative transfer models, Atmos. Chem. Phys., 7, 1809-1833, 2007.

7. Contact

For any questions, comments or bug report regarding the O_3 AMF LUT, please contact François Hendrick at the Belgian Institute for Space Aeronomy (IASB-BIRA).
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8. Acknowledgments

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9. Supplementary material

The following data files are provided together with the present document:

File name	Description
o3_amf_lut_v2_0.zip	O_3 AMF LUT package. This contains AMF LUTs provided in 18 latitude bands, monthly tables of global albedo values and an AMF extraction routine. The source code is given together with MS-DOS executable files.
ndacc_xsecs_v2.zip	Zip file containing reference NO_2, O_3, H_2O, O_4 and Ring effect absorption cross-sections recommended for use in DOAS ozone retrievals.