Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations

FRM$_4$DOAS

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NDACC MAX-DOAS instrument certification procedures document

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1 Introduction

This Deliverable D18-v2 presents the final version (April 2020) of the NDACC Appendix VII document and the current status of NDACC affiliation for FRM_4DOAS partners stations. The NDACC Appendix VII describes the general guidelines for NDACC UV/vis zenith-sky and MAX-DOAS instruments operation and data analysis. It includes the most updated recommendations and quality criteria for the certification of new UV/vis spectrometers within NDACC.

2 FRM_4DOAS: Procedure and status of NDACC affiliations

The NDACC affiliation procedure for FRM_4DOAS partners stations is based on the following two-step approach:

1) Official demand for affiliation should be sent by instrument PIs to NDACC UV/VIS WG co-chairs
2) Instrument certification procedure:
    - *Full procedure :*
        - New instrument(s) from non-affiliated PIs
        - New site(s) and/or new instrument(s) from already affiliated Pis
        - New affiliated PIs engage to participate to next intercomparison campaign
    - *Simplified procedure (automatic qualification):*
        - MAX-DOAS instrument(s) already affiliated for zenith-sky products, from PI having successfully participated to a past NDACC MAX-DOAS intercomparison campaign

The current status of the affiliation procedure for FRM_4DOAS partners stations is summarized in the following table:

Xianghe	NA	N	MAX-DOAS	BIRA-IASB/IAP	Michel Van Roozendael/Pucai Wang
Uccle La Reunion	NA NA	Y Y	Pandora MAX-DOAS	BIRA-IASB	Michel Van Roozendael
Harestua	A	--	ZSL-DOAS	BIRA-IASB	Van Roozendael
Ny-Alesund	A	--	MAX-DOAS	Bremen	John Burrows/ Andreas Richter
Izana	A	--	MAX-DOAS	INTA	Margarita Yela
Bremen Athens	NA NA	Y Y	MAX-DOAS MAX-DOAS	Bremen	John Burrows/ Andreas Richter
De Bilt	NA	Y	EnviMes	KNMI	Ankie Piters
Mainz	NA	N	Tube-DOAS	MPIC-Mainz	Thomas Wagner
Lauder	NA	Y	EnviMes	NIWA	Richard Querel
Neumayer	A	--	MAX-DOAS	U. Heidelberg	Udo Friess
Heidelberg Arrival Height	NA NA	Y Y	MAX-DOAS MAX-DOAS	U. Heidelberg	Udo Friess
Thessaloniki	NA	Y	Phaeton	AUTH	Alkis Bais

NA=Not affiliated; A=Affiliated
Color codes: green (to be affiliated), blue (already affiliated), orange (no affiliation planned in the short term)

The affiliation of the above instruments started during this CCN02 and will be finalised during the new CCN03.

Appendix VII

Protocol for NDACC UV/Vis instrument operation and data analysis

April 2020

1. Introduction

Introduced in the late seventies, passive ultraviolet and visible (UV/Vis) spectroscopy using scattered sunlight as a source has been developed into a powerful technique for unattended long-term monitoring of atmospheric composition in both the stratosphere and the troposphere. The UV/Vis technique has been part of the NDACC observation system since the inception of the network in the early nineties. One of its key advantages is to allow automated daily measurements of stratospheric gases (NO_2, O_3, BrO, OClO) even under cloudy conditions. Such measurements have been conducted for several decades and used for trend analysis, assessment of global chemistry-transport models and validation of a number of atmospheric composition satellite missions such as the NASA TOMS series, Aura/OMI, ERS-2/GOME, ENVISAT/SCIAMACHY, and the successive GOME-2 and IASI instruments on EUMETSAT METOP 1-3.

More recently in the early 2000s, the UV/Vis zenith-sky twilight technique has been extended to allow for vertically resolved measurements of the tropospheric composition using the Multi-Axis DOAS (MAX-DOAS) technique. This addition in measurement capability allows NDACC to expand further from its original emphasis on stratospheric and total column data products to include tropospheric observations e.g. such as tropospheric NO_2 and HCHO for pollution monitoring.

Various research studies have demonstrated the capacity of the MAX-DOAS technique to derive low-resolution vertical profiles of several tropospheric species such as NO_2, HCHO, CHOCHO, HONO, SO_2, BrO, IO, H_2O, O_3 as well as aerosol extinction. Among these species, NO_2 and HCHO have reached high maturity and are being measured by a growing number of instruments. Some of them have provided data to the Rapid Delivery data base of NDACC for several years. The formal integration of MAX-DOAS NO_2 and HCHO tropospheric profile measurements within NDACC in addition to the historical stratospheric column data products (NO_2 and O_3) is under way.

The present document describes the validation process for new UV/Vis zenith-sky and MAX-DOAS instruments, as well as the criteria for maintaining data quality from existing instruments. Measurement certification criteria are established for slant column abundances of NO_2, O_3, BrO, HCHO and O_4. The latter molecule (collisional dimer of oxygen) is used as part of the MAX-DOAS inversion process and provides information on aerosol extinction.

2. Quality criteria for the evaluation of new zenith-sky and MAX-DOAS instruments and instrument teams

The emphasis within NDACC is on the long-term monitoring of the atmospheric composition, which requires a dedicated approach to the maintenance of the quality of the measurements and the archiving of data. The ability to determine long-term trends imposes strong requirements on instrument stability and calibration maintenance, which in turn implies the need for operators having a thorough understanding of the measurement technique.

The accuracy of UV/Vis data products is determined by the following key factors:

(1) The slant column measurement accuracy and precision (generally expressed in terms of systematic and random uncertainties). These are primarily determined by instrumental factors, calibration procedures and spectral retrieval methods, but also depend on the accuracy of the molecular absorption cross-sections used in the retrieval process.

(2) The accuracy of vertical column and/or vertical distribution profile retrieval, which depend (a) on the accuracy of the slant column measurements used as input, (b) the suitability and accuracy of radiative transport models used to calculate the air mass factors (AMFs) needed in the inversion process, (c) the choice of the atmospheric data bases and other ancillary data used as input and a priori (e.g. atmospheric temperature, pressure and ozone profiles), and (d) the suitability of the inversion methods used to convert slant column measurements into final column and/or profile data products.

(3) The suitability of filtering methods used to identify and flag (or exclude) erroneous data due to e.g. cloud contamination, instrumental artefacts, field of view obstruction affecting the measurement noise, etc.

For total column measurements of NO_2 and ozone using the zenith-sky geometry, the limiting accuracy of instruments operating at clean sites is generally driven by uncertainties in AMF calculations (which depend on (2b) and (2c) above) and by the estimation of the residual amount in the reference spectrum.

For MAX-DOAS measurements of tropospheric species, uncertainties are more complex to establish and related to a number of parameters such as a-priori profiles, covariance matrices of both measurement and a-priori data, aerosol content and aerosol type.

The process of certifying a new UV/Vis observing system for NDACC involves two major steps:

1) An evaluation of the instrument design, the available data analysis tools and the expertise from the instrument team (as detailed in Section 2.1 below) and
2) the formal and successful participation in a blind or semi-blind instrument intercomparison campaign (as detailed in Section 2.2 below).

Full certification is granted to instruments and measuring groups that fulfil a set of general and specific criteria as described in Section 2.3.

2.1 Evaluation of instrument design, data analysis tools and expertise from the measuring team

Before a new candidate instrument is considered for certification within NDACC, the group responsible for instrument operation may be asked (upon decision of the UV-Vis working group (WG) co-chairs) to supply the following to the NDACC UV/Vis WG representatives:

- A detailed technical description of the instrument including detection limits of trace gas slant columns (or S/N ratio of spectra in key wavelength regions) and general operating parameters.
- An outline of the spectral analysis technique used with details of the retrieval code used, in particular the wavelength calibration procedure applied, and a description of any deviation with respect to NDACC recommended settings (e.g. source of absorption cross-sections or fitting interval).
- An example of raw measured spectra for inspection by the WG co-chairs. Typically, this will consist in one full day of observations under standard operating conditions, covering both noon and twilight.
- A report on the instrumental calibration performed by the team. Ideally, this shall cover the instrumental spectral response function (ISRF), dark current and electronic offset spectra, detector linearity response, an estimate of the stray light levels and the instrument polarisation characteristics. For MAX-DOAS instruments, a description of the method used to assess the accuracy of the elevation pointing and the instrumental field of view will have to be provided as well. Note that recommendations on how to perform these calibrations are given in a MAX-DOAS Best Practice Document, available on the UV/Vis WG web site (see Section 4).
- Examples of existing measurement data in support of the evaluation process, e.g. results from local intercomparisons, scientific publications involving validation activities or equivalent reference data.

Discussions and data exchange between the PI and the UV/Vis WG representatives may be required, as the WG must be satisfied with this part of the evaluation.

2.2 Instrument intercalibration field campaign

Instrument intercomparison field campaigns are regularly organised, at the frequency of approximately one campaign every 5 years. Table 1 lists the NDACC UV/Vis intercomparison campaigns that have been organised since the inception of NDACC. The aim of such campaigns is to provide an opportunity for certification of new groups but also to foster interactions between groups and promote scientific improvements.

Table 1 : NDACC UV/Vis intercomparison campaigns

Date	Location	Name and affiliation of campaign referee	References
May 12-23, 1992	Lauder, New-Zealand	David Hofmann, NOAA, USA	Hofmann et al., 1995
June 11-21, 1996	Observatoire de Haute Provence, France	Howard Roscoe, BAS, UK	Roscoe et al., 1999; Aliwell et al., 2002

February 13 to March 8, 2003	Andoya, Norway	Anne-Carine Vandaele, BIRA-IASB, Belgium	Vandaele et al., 2005
June 15-30, 2009	Cabauw, The Netherlands	Howard Roscoe BAS, UK	Roscoe et al., 2010; Piters et al., 2012; Pinardi et al., 2013; Friess et al., 2016
September 12-18, 2016	Cabauw, The Netherlands	Karin Kreher, BK Scientific GmbH, Germany	Kreher et al., 2019; Donner et al., 2020; Tirpitz et al., 2020

The certification of a new instrument relies on the successful participation in an intercomparison of measurements and data analysis following the "semi-blind" rules detailed below. New instruments are evaluated by comparison with already certified instruments under the supervision of an impartial campaign referee. The intercomparison should adhere to the following conditions:

- The intercomparison is conducted at a site selected to allow for successful observations of the target data products under a wide range of concentration values and under both clear and cloudy conditions.
- The intercomparison is conducted for a period of not less than 10 days, tentatively with all instruments operating correctly.
- Measurements taken by all participating instruments are made over the whole day with a period of high temporal sampling near midday, each day of the intercomparison irrespective of experienced weather conditions. For MAX-DOAS instruments, measurements should cover a minimum of 10 different elevation angle values (extending from the lowest possible elevation to the zenith) in at least one common azimuth direction. For twilight measurements, the integration period should be less than the time taken for a 1° change of solar zenith angle (5 minutes at mid-latitudes) or a maximum of 5 minutes for extreme solar zenith angle values.
- Measurements taken by all the participating instruments should be coincident in time to better than one minute, to minimize interpolation errors when performing comparisons. For MAX-DOAS instruments, the same measurement protocol should be adopted, at least in the common azimuth direction.
- For MAX-DOAS instruments, scans of the horizon should be performed daily at noon by all participating instruments. This procedure allows to verify the stability and regularity of the elevation pointing.
- The wavelength interval used for data processing of all the target species should be the same for all the participating instruments. Non-standard wavelength intervals might have to be selected to fulfill this important requirement.
- The cross-sections used in the analysis must be from the same source (specified ahead of the campaign), and appropriately convolved to each instrument's resolution, or a slit function determined by spectral fit, when this is shown to be a good approximation for the measured slit function.
- If the key calibration characteristics (dark current, detector linearity, signal to noise ratio at given integration time and illumination level, spectral stray-light, slit function,

polarization response and, for MAX-DOAS instruments, telescope field of view and accuracy of elevation pointing) are not supplied by the PI of an instrument being evaluated, they must be measured during or prior to the intercomparison according to protocols to be established.

- Unless otherwise specified by the campaign referee, the data analysis should provide at least two sets of results: (1) A data set analysed using a daily selected midday reference spectrum, to be submitted to the referee normally within 1 day of the measurements and (2) another data set analysed using a single midday reference spectrum for the whole intercomparison data set to be submitted to the referee within a maximum of three months of the end of the intercomparison campaign. For MAX-DOAS instruments, an additional data set analysed using sequential reference spectra (preferably interpolated at the time of each individual off-axis measurement) selected for each elevation scan might have to be delivered. Final "polished" results will be submitted within a maximum of four months of the end of the intercomparison campaign.
- Blindness rules are important for an instrument evaluation, since the goal is to provide evaluations that represent a "true picture" of each instrument performance. However, experience has shown that campaign results strongly benefit from the adoption of a "semi-blind" intercomparison protocol where preliminary data submitted by participants can be displayed by the referee during the campaign in a form that does not enable participants to identify individual instruments. Experience has also shown that displays of data that do not identify groups (but enable participants to see the general form of the others' measurements) were found to not compromise the integrity of the intercomparison. This approach is therefore recommended for use in UV/Vis intercomparison campaigns. Note that individual results being evaluated must not be exchanged between any participants until final results are submitted by all instrument groups.

2.3 Acceptance criteria for new instruments

The UV/Vis WG or its designated representative(s) will examine the results of the intercomparison and make a recommendation to the NDACC Steering Committee. While additional factors may possibly be examined, the following points are considered as general criteria for acceptance:

- The calibration report provided by instrument PIs (or determined prior to the intercomparison) must be analysed and endorsed by the UV/Vis co-chairs.
- Good consistency between the results obtained using the daily reference spectrum and the results obtained using the campaign single midday reference spectrum. This helps identify problems caused by long period (10 day) drifts in the instrument function or spectral wavelength repeatability. The reference instrument errors can be used as a guide for acceptance.
- For zenith-sky measurements performed at twilight:
    - Good result self-consistency: This can be assessed by examining the "smoothness" of the twilight data series. At clean sites, midday result variations should remain small, < $1x10^{15}$ cm^{-2} for NO_2, < $1x10^{18}$ cm^{-2} for ozone and < $3x10^{13}$ cm^{-2} for BrO slant columns.

- Acceptable signal to noise of the order of 500 or better at high (up to 92° for spectra in the visible) and small solar zenith angles. This can be estimated by examining residual spectra.

- For MAX-DOAS measurements performed during the day at small and moderate (< 85°) solar zenith angles:
  - Acceptable signal to noise of the order of 1000 or better should be reached in spectral ranges relevant for the retrieval of the target species.
  - Horizon scans performed over the duration of the campaign (during days of good visibility) should display an acceptable level of stability and regularity to within a few 10^{th} of a degree in elevation.

In addition to these general criteria, measurable criteria for the certification of the zenith-sky and MAX-DOAS primary slant column data products, i.e. NO_2, O_3, HCHO and O_4 differential slant column measurements, have been formalised based on results from previous intercomparison exercises (see Table 1 and, in particular, Kreher et al., 2019 for details).

Because no absolute calibration is possible, accuracy is determined by quantifying the consistency of each instrument relative to a designated reference data set, which is generally obtained from the median of a series of instruments identified as being consistent within their mutual uncertainties (see below). Spectral measurements made during the intercomparison period are analysed by all participants using agreed evaluation settings (wavelength interval, cross-sections, etc.) to obtain individual comparison results. A reliable method to determine which instruments meet a certification is a regression analysis where all combinations of the sets of measurements are intercompared. Matrices of linear regression residual RMS error, slope and intercept are generated in order to identify the instruments that agree most closely. After suitable averaging (median might be preferred over averaging to minimise the impact of possible outliers), the results from these instruments can then be used as a reference for comparing the results of the other participating instruments.

Experience from previous intercomparison campaigns, especially the most recent intercalibration organised in Cabauw, The Netherlands, September 2016 (see Table 1), has been the basis for choosing the numbers listed in Table 2 as acceptance criteria for NO_2, O_3, HCHO and O_4 measuring instruments. Details on the method used to define these numbers are given in Kreher et al. (2019). Note that common acceptance criteria are being used for slant column measurements from zenith-sky and MAX-DOAS instruments.

Table 2 : Acceptance criteria for NDACC measurements of NO_2, O_3, BrO, HCHO and O_4 slant columns

Trace gas species	Spectral interval (nm)	Acceptance criteria for slant column measurements		
		Slope	Intercept (molec/cm²)	RMS residual (molec/cm²)
NO_2	425 – 490	1.00 ± 0.05	1.5 1015	8.0 10^{15}
	411 – 445	1.00 ± 0.05	1.5 10^{15}	8.0 10^{15}
	338 – 370	1.00 ± 0.06	2.0 10^{15}	1.0 10^{16}
O_3	450 – 520	1.00 ± 0.04	2.0 10^{17}	1.0 10^{18}

	320 – 340	1.00 ± 0.04	$1.0\ 10^{18}$	$4.0\ 10^{18}$
HCHO	336.5 – 359	1.00 ± 0.10	$5.0\ 10^{15}$	$1.0\ 10^{16}$
O_4 (*)	425 – 490	1.00 ± 0.05	$7.0\ 10^{41}$	$3.0\ 10^{42}$
	338 – 370	1.00 ± 0.06	$8.0\ 10^{41}$	$3.0\ 10^{42}$

(*) Note: the units for O_4 slant column measurements are molec^2/cm^5

Groups with intercomparison results that meet these accuracy criteria together with the general acceptance criteria (see above) are certified for NDACC UV/Vis observations. Note that these specifications are not to be taken as rigid criteria. Some groups may have instruments that produce results that are close to these figures. In such case, certification might still be awarded by the UV/Vis working group co-chairs recognising the potential and usefulness of such instruments for NDACC. In this case, assistance will be offered to improve measurement accuracy and eventually prepare a participation to the following intercomparison.

For the special case of BrO, no acceptance criteria can be derived from previous campaigns due to a lack of comparison data. For this particular molecule, acceptance is only based on analysis of the measurement self-consistency and on the quality of the scientific material provided in support of the application.

3. Quality criteria for the evaluation of continuously operated zenith-sky and MAX-DOAS instruments

The NDACC instrument PI is responsible for maintaining data quality from his/her instrument on a continuous long-term basis. This should include routine procedures on how to check on instrument performance (e.g. stray light monitoring, instrument resolution tests, error figure monitoring and residual spectra checks) and how to deal with instrumental upgrades or replacements necessary to maintain high data quality standards.

3.1 Routine operation of an NDACC certified instrument

The investigator must secure suitable instrument operation and maintenance records. A brief station report requesting this information as part of a prescribed format has to be submitted once a year. Repairs and changes to equipment must be appropriately logged as well as calibrations made afterwards to identify any changes in accuracy. Meta data information also needs to be updated regularly on the NDACC data base and any changes need to be reported as part of this meta data file as well.

Where available, the investigator should use data from other instruments at the measurement site to compare with their UV/Vis measurements, for example Dobson, Brewer, Sonde and Lidar data for ozone total column comparisons. Additionally, the use of more than one UV/Vis instrument operated simultaneously at the same site for a reasonable period of time (a couple of months at least) and the subsequent comparison of results also offer a higher level of confidence in the data.

The investigator must maintain a routine data archiving procedure. The maximum time between measurement and data submission to the NDACC data base should not exceed 12 months but a more frequent data submission is encouraged. When submitting data, the GEOMS HDF4 data format prescribed for use within NDACC should be adopted (see https://avdc.gsfc.nasa.gov/index.php?site=1876901039). A facility to deliver unconsolidated data is offered through the Rapid Delivery repository, which is used as a service in support of validation activities (e.g. for satellite missions or the EU Copernicus Atmospheric Monitoring Service). Investigators are encouraged to contribute to this service.

When equipment problems compromise data continuity or quality, the investigator should inform the NDACC UV/Vis working group. Similarly, if the operation of an NDACC instrument or a station is in danger of being interrupted or discontinued (e.g. due to loss of funding), this should be brought to the attention of the UV/Vis working group co-chairs and to the NDACC steering committee.

The instrument PI or members of her/his group must be willing to participate in intercomparison exercises if financially feasible. Because of the effort and cost of such campaigns, these are organized at the frequency of about one campaign every 5 years. This allows for full exploitation of each intercomparison exercise and for significant updates in the objective and scope of successive campaigns, according to scientific progress and the evolution of NDACC.

Approximately every 1-2 years, the NDACC UV/Vis working group and community holds a workshop to discuss new research results as well as ways of improving measurement and analysis quality. Groups experience changes in instrument operators (or responsible scientists) occasionally, and knowledge within the UV/Vis community that workshops provide is an excellent way of providing training for new people. Workshops also foster ongoing collaboration between groups, which helps to ensure high measurement quality standards within the NDACC UV/Vis community.

3.2 Upgrade or replacement of an NDACC certified instrument

Instrument and analysis improvements that enhance scientific output or data quality are encouraged. The group should ensure, however, that data continuity and quality is maintained. Where possible, an improved instrument should be operated in parallel with the existing instrument for a period of at least 6 months, and the data should be carefully compared before switching over to the new instrument. When an instrument or analysis technique improvement results in a change in the measurement results, this must be fully reported and recorded in the archive as part of the metadata record.

4. Standardised instrument operation and data retrieval

Recommendations for standardized instrument operation and data retrieval have been agreed upon as part of activities of the UV/Vis working group. It is the responsibility of the instrument PI to make sure that these recommendations are properly implemented and used for the production of data to be archived in the NDACC data base. PIs are strongly encouraged to consult the following documents at the NDACC UV/Vis working group web site:

- NDACC UV/Vis Best Practices Document
- NDACC UV/Vis Algorithm Theoretical Background Document
- NDACC UV/Vis Recommended Retrieval Settings

5. NDACC UV/VIS Central Processing

In addition to recommendations for standardized data retrieval of UV/Vis zenith-sky and MAX-DOAS data products, the UV/Vis working group has developed under an ESA-funded project (FRM$_4$DOAS) a Central Processing System (CPS) operated at BIRA-IASB and accessible to NDACC certified instrument PIs. The current version of the CPS is designed to ingest level-1 spectral measurements from MAX-DOAS instruments and generate the following level-2 data products in fast-delivery mode:

- Vertical profiles and integrated columns of tropospheric NO_2 and HCHO
- Vertical profiles of aerosol extinction and aerosol optical density at O_4 absorption wavelengths
- Vertical profiles and integrated columns of stratospheric NO_2
- Total ozone vertical columns.

These products are generated using standard retrieval algorithms selected through a Round-Robin intercomparison, or based on well-established algorithms published in the peer-reviewed literature. The UV/Vis CPS is fully documented on the FRM4DOAS project site (see http://frm4doas.aeronomie.be)

Upon successful registration, access to the CPS on a dedicated incoming ftp server requires the adoption of a common standardised level-1 netCDF data format also described on the FRM$_4$DOAS project web-site. Once being ingested, level-1 data files undergo QA/QC and subsequent processing for the data products listed above to produce final level-2 products. These are delivered in (1) an internal netCDF file format that contains a complete and fully traceable set of variables and ancillary data information, and (2) the standard GEOMS HDF4 file format (see https://avdc.gsfc.nasa.gov/index.php?site=1876901039), suitable for submission to the NDACC Rapid Delivery data base. GEOMS HDF4 files are automatically transferred to the EVDC databases for duplication. The access to the internal (master) netCDF output files is currently restricted to instrument data providers. Various services are implemented within the CPS to allow for the detection of anomalies in the processing chain and generate various reports (status on processed files, statistics, list of anomalies, etc). Upon detection of anomalies, e-mail alerts are sent to the corresponding data providers.

Initiated in July 2016, the UV/Vis CPS will begin operation by spring 2020 using an initial set of 11 stations. These will progressively be expanded as part of the follow-up activities of the ESA FRM$_4$DOAS project. The system is primarily designed to allow for automated and quality-controlled MAX-DOAS processing in rapid-delivery mode to serve the validation of satellite missions such as Sentinel-5 Precursor and the future Sentinel-4 and Sentinel-5. In addition, it will generate optimized quality-controlled off-line data products ready for feeding the NDACC consolidated data base. Facilities to reprocess long-term data series at relevant sites are also part of the Service.

More details about the FRM$_4$DOAS project can be found at http://frm4doas.aeronomie.be/index.php.

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