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

FRM_4DOAS

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MAXDOAS Network Scientific Requirements

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Content

1 Introduction

The Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations (FRM_4DOAS, see http://frm4doas.aeronomie.be/) is a 2-year ESA project which started in July 2016. It aims at further harmonization of MAXDOAS systems and data sets, through the

- specification of best practices for instrument operation
- demonstration of a centralised NRT (near-real-time/6-24h latency) processing system for MAXDOAS instruments operated within the international Network for the Detection of Atmospheric Composition Change (NDACC)
- establishment of links with other UV-Visible instrument networks, e.g. Pandonia

While the project itself is limited to tropospheric and stratospheric NO_2 vertical profiles, total O_3 columns, and tropospheric HCHO profiles from a small number of stations, the aim is to collect and create the necessary information, guidelines and infrastructure which can be the basis for a network including many more MAXDOAS instruments and covering all MAXDOAS products.

In this document, the basic considerations for layout and design of network, instruments, data evaluation, and quality control and assurance are outlined for a MAXDOAS network for fiducial satellite validation measurements.

2 Validation needs addressed by MAXDOAS measurements

MAXDOAS instruments can provide tropospheric and stratospheric measurements of a number of trace gases relevant to Montreal Protocol monitoring, air quality and pollution research. Because of the similarity in the measurement principle, they can cover most of the data products of UV/visible satellite instruments, including NO_2, HCHO, SO_2, glyoxal, and ozone. Through the use of the MAXDOAS measurement geometry, total and tropospheric columns can be derived, either using only the 30° and 90° elevation observations and a standard air mass factor (AMF) approach or by using additional observations taken at small elevation angles and applying a profile inversion algorithm. By extending measurements to twilight conditions, information on the stratospheric vertical distribution of some trace gases (NO_2, O_3, BrO, OClO) can be obtained by applying profile inversion algorithms using the change of vertical measurement sensitivity with solar zenith angle (SZA).

Because of the geometry of observation in MAXDOAS mode, the tropospheric light path length is of the order of a few km if only the 30° elevation measurement is used, and 5 – 20 km for the profiling measurements based on the lowest elevations. As photons from many different light paths contribute to the signal observed at the instrument, one can conceive the averaging volume as a relatively narrow slice of several kilometres length, and oriented in viewing direction. In this direction, the volume is comparable to (and often even larger than) the ground-pixel size of the next generation of satellite instruments. For full representativity of a satellite observation, measurements in several azimuthal directions are needed as they are now routinely taken by many MAX-DOAS instruments.

Stratospheric measurements, being performed at twilight, are typically representative for much larger horizontal areas (a few hundreds of kilometres in the stratosphere), which is generally compatible with the natural horizontal variability of stratospheric species (see http://nors.aeronomie.be/projectdir/PDF/D4.4_NORS_SR.pdf for an overview on the horizontal representativeness of zenith-sky twilight DOAS and MAXDOAS measurements).

While column measurements can directly be used in operational validation, the tropospheric vertical profiles, which can be derived if more elevation angles are used, can also serve as validation of the a priori trace gas profiles used in the satellite data analysis. The latter might not become part of an automated validation process but will provide highly relevant information for understanding satellite data uncertainties, especially on the AMF-related part of the retrieval. They also enable application of averaging kernels resulting in more quantitative comparisons between satellite and ground-based observations.

3 Accuracy requirements for satellite data product validation

Table 1 presents an overview of the accuracy requirements for air quality satellite measurements as determined in the framework of the Copernicus Sentinel 5 Precursor mission (see https://sentinels.copernicus.eu/documents/247904/2506504/S5P-Level-1b-L2-numbered-validation-requirements.pdf). Although these requirements will not be matched by actual satellite sensors in all cases, they provide a reference in terms of accuracy requirements for validation data. The last column of Table 1, presents an estimate of the typical accuracy achievable using ground-based DOAS and MAXDOAS instruments. The values listed here have been extracted from the recent peer-reviewed literature (see Table 1). They will be further refined and discussed as part of the activities of the FRM$_4$DOAS project.

Table 1. Accuracy requirements for satellite measurements and corresponding accuracy estimates for DOAS and MAXDOAS measurements (based on the literature).

Species	Data Product	Accuracy requirements for satellite measurements	Theme	Accuracy of DOAS/MAXDOAS measurements
Ozone	Total column	3.5-5%	A3/B1	5% (Hendrick et al., 2011)
NO2	Stratospheric column	<10%	A3	<10% (Hendrick et al., 2004)
	Tropospheric column	25-50%	B1/B3	15% (Hendrick et al., 2014; Vlemmix et al., 2011)
HCHO	Tropospheric column	40-80%	B1/B3	20% (Franco et al., 2015; Vigouroux et al., 2009).
SO2	Enhanced stratospheric column	30-50%	A3	--
	Tropospheric column	30-50%	B1/B3	25% (Wang et al., 2014)
Glyoxal	Tropospheric column	1.2e14 molec/cm^2 or 60%	B1	30% (Sinreich et al., 2010; Mahajan et al., 2014).

A3 – Ozone layer assessment
B1 – Air quality protocol monitoring
B3 – Air quality assessment

4 Network layout requirements

The geographical layout of an optimal MAXDOAS validation network is determined by the spatial variability and distribution of the parameters of interest. Species with long atmospheric lifetime, such as CO_2, need fewer stations than reactive gases such as NO_2. Thorough validation requires a spatial distribution of the measurements covering:

- Both hemispheres
- All relevant latitudes from the tropics to polar regions
- Background regions and sites where high concentrations are expected
- Regions having different conditions with respect to parameters which can potentially affect measurement quality such as albedo, cloud cover, aerosol loading, topography

Which regions to target for appropriate sampling of the range of measurement values depends on the trace gas or measurement quantity of interest. An overview of relevant regions is shown in Table 2.

Ideally, the measurement locations should be chosen to provide data representative for an area of the size of the satellite pixel or larger. For UV/vis instruments before the 'Sentinel-era', this is difficult for several reasons – because of atmospheric and surface variability but also because of the large volume of air contributing to an individual satellite measurement. The satellite pixel size has decreased in recent years and will be even smaller for future missions, making it easier to find stations representative for a full satellite pixel and also finding satellite pixels measuring a similar quantity as the ground-based observation. For small satellite pixels (e.g. 3.5 x 7km² of the TROPOMI instrument), the spatial averaging by MAXDOAS observations (5 – 20 km) may become a limiting factor. Also, spatial gradients close to emission regions are often large, so mapping the hot-spots and measuring values representative for larger areas is often in contradiction.

Validation measurements for volcanic SO_2 have in some respect different requirements than other observations. Because of the unpredictable nature of volcanic emissions, it makes sense to have several instruments located around a potential volcanic source, ideally also at different distances. This increases the probability to actually have validation measurements available in case of an emission event. As in some places anthropogenic and volcanic signals are both present and therefore mixed in the satellite data, a combination of instruments close to industrial / power plant sources and volcanic emissions might be needed.

Table 2: Regions of interest for satellite validation measurements

Species	Background	Hot spot
NO_2	• Rural areas on all continents • Oceanic areas	• Industrial areas on all continents • Shipping regions • Biomass burning areas in Europe, South America, Africa, Asia • Soil emission areas (Savannah, agricultural areas) • Lightning regions, if possible separated from other sources
Formaldehyde and Glyoxal	• Sparsely vegetated area • Oceanic regions • Desert regions	• Biogenic emission regions (boreal forests, rain forests) • Biomass burning areas in Europe, America, Africa, Asia • Industrial hotspots (Po valley, PRD, Houston area, ..) • Continental outflow areas
SO_2	• Rural areas • Oceanic regions	• Volcanic emission regions (degassing + explosive) • Industrial hot spots (ore mining, power plants, shipping regions) • Oil and gas production regions
Ozone	• Rural regions • Oceanic regions • Polar regions (ozone depletion events)	• Biomass burning regions • Continental outflow regions • Industrial regions

The considerations listed above apply mainly for an operational validation network. It has to be complemented by validation campaigns providing data from additional instruments and also moving platforms in order to better characterize spatial gradients or for example the latitudinal distribution. For MAXDOAS measurements in particular, the nature of the network (a heterogeneous network of different instruments funded and operated by various institutes and universities) limits the applicability of the criteria listed in Table 2 as only part of the instruments are deployed with satellite validation being the main application target.

5 Instrument requirements

Instrument requirements for MAXDOAS instruments to be used in satellite validation networks are driven by the requirements on the quantities measured by the satellite, both in terms of the relevance of these quantities and in terms of the necessary precision and accuracy. In many cases, a combined measurement of all relevant quantities is useful as this makes best use of a given infrastructure. Exceptions are monitors for volcanic emissions or other measurements in remote regions such as the Arctic having limited access to shelter, power, and data bandwidth where simple instruments provide advantages.

Some aspects to be taken into account when evaluating instrument requirements are:

- Does the wavelength coverage allow measurement of all species of interest?
- Does the signal to noise ratio (SNR) allow measurement uncertainties low enough to provide meaningful validation for satellite observations?
- Does the instrument perform measurements at different elevation angles in order to separate tropospheric and stratospheric column amounts?
- Are pointing accuracy and FOV good enough to enable profile inversion?
- Can measurements be performed at different azimuth angles to evaluate horizontal gradients?

An overview on qualitative requirements for some instrumental parameters is given in Table 3. These values are based on experience and should not be seen as quantitative threshold requirements. With respect to the signal to noise ratio, the target should be 3000 – 4000, and if this is not reached, integration time should be increased until the SNR is good enough. This is of particular relevance for tropospheric columns calculated using the 30° elevation angle measurement as in this case, the difference in AMF to the zenith measurement is small (ΔAMF = 1).

Table 3: MAXDOAS Instrument requirements for satellite validation measurements.

	NO_2	HCHO	Glyoxal	SO_2	O_3 UV	O_3 Visible*
Wavelength coverage [nm]	400 – 500	340 – 360	400 – 500	305 – 330	320 – 350	450 - 550
Spectral resolution	< 1 nm	< 0.6nm	< 1 nm	< 0.5 nm	< 0.8 nm	< 1nm
SNR	3000 - 4000	4000	4000	3000	3000	3000 - 4000
Elevation angles trop. Columns	30°, 90°					
Elevation angles profiles	1°, 3°, 5°, 10°, 30°, 90°					
Elevation accuracy profiles	<= 0.2°					
FOV	<= 1.5°					
Solar zenith angles to be covered in twilight geometry	75° – 94°					

* Total column from zenith twilight observations

Instrument requirements as given in the table are only indicative – for example, NO_2 can also be retrieved from measurements in other spectral regions, a different set of elevation angles can also be used for profiling and for tropospheric columns, 20° as well as 30° elevation can be used.

6 Operation requirements

For operational validation, data is needed in a reliable and traceable way which includes instrument configuration, measurement protocol, calibration / characterisation procedures, data evaluation and data delivery (see for example http://frm4doas.aeronomie.be/). For the heterogeneous MAXDOAS network, a centralised calibration and processing unit as it is being developed in the FRM_4DOAS project will help to better achieve these requirements without putting too much burden on the individual station operators.

Main aspects relevant for operations of MAXDOAS instruments to be used for operational validation are described below.

6.1 Instrument operation

- Measurement time and frequency need to be adapted to satellite overpasses. For tropospheric measurements, time differences of less than 30 minutes are preferable which translates into the need to have measurements at intervals of 15 – 30 minutes throughout the time periods of satellite overpasses or better the full day. The acceptable time difference depends on typical horizontal gradients in combination with wind speed and can be longer in background regions.
- In order to continuously monitor instrument performance, several characterisation measurements should be performed on a regular basis (ideally daily but at least monthly). These include
  - Horizon scans to monitor pointing accuracy and FOV
  - Dark signal measurements to monitor dark current and electronic offset
  - Line lamp measurements to characterize instrument spectral response function (ISRF)
- Visual inspections of instrument (when having operators at the station), measurement results and QA reports needs to be performed on a regular basis (at least monthly) in order to identify and solve problems in a timely manner. Guidelines for such analyses are given in the MAXDOAS Calibration and Operations Best Practice document (http://frm4doas.aeronomie.be/ProjectDir/Deliverables/FRM4DOAS_D4_MAXDOAS_Best_Practices.pdf) and will be provided through the FRM4DOAS webpage.
- Special attention needs to be given to recording the accurate time of measurement, for example by synchronizing instrument clocks with GPS or time servers via internet.

- Instruments (or in the case of multiple identical instruments at least one of the instrument types) should participate regularly in the semi-blind intercomparison campaigns organised by NDACC.

6.2 Data evaluation

- Standardized and automated QA tests have to be performed on the data together with data analysis in order to monitor instrument performance and flag poor data. While this will be performed automatically in the centralised FRM_4DOAS processing system, the recommended tests are also discussed in MAXDOAS Calibration and Operations Best Practice document provided through the FRM_4DOAS webpage (http://frm4doas.aeronomie.be/ProjectDir/Deliverables/FRM4DOAS_D4_MAXDOAS_Best_Practices.pdf).

- Data evaluation has to be performed daily and in an automated way to minimise latency in data delivery to the satellite validation facility.

- DOAS data evaluation has to follow standard settings as defined within the Network for the Detection of Atmospheric Composition Change (NDACC, see http://ndacc-uvvis-wg.aeronomie.be/tools.php) in order to ensure inter-comparability of measurements from different stations. This includes recommendations on fitting ranges, cross-sections and corrections applied. Settings for O_3 and NO_2 in the visible range can be found at http://ndacc-uvvis-wg.aeronomie.be/tools.php. Alternatively, processing can be done in a centralised facility to which radiances measured by the network instruments are submitted. This is the approach taken in the FRM_4DOAS centralised processing facility, which aims at including processing from level 1 data to slant columns to vertical columns and profiles in combination with automated quality assurance and control. This is achieved by monitoring, reporting and accounting for instrument parameters such as signal to noise ratio, instrument spectral response function, wavelength stability and other quantities throughout the processing. As a result, data products are as uniform as possible and are accompanied by standardized information on data quality, e.g. a dedicated QA/QC and cloud flagging approach.

6.3 Data delivery

- Data delivery should be daily and automated to ensure regular submissions

- Data delivered should include the main measurement quantities, uncertainty information and quality flags as well as metadata

- Data formats should follow the GEOMS standards (see next section).

7 Data format requirements

MAXDOAS level-2 data should be reported in the GEOMS (Generic Earth Observations Metadata Standard) UVVIS.DOAS HDF format. This has been developed during the FP7 NORS project (see http://nors.aeronomie.be/projectdir/PDF/NORS_D4.1_DFD.pdf) for reporting level-2 UV-vis data in off-axis (trace gas + aerosols), zenith, and direct-sun viewing geometries. Corresponding templates and guidelines for file creation are described on the AVDC website (http://avdc.gsfc.nasa.gov/index.php?site=1876901039). The added value of the GEOMS HDF format resides in the possibility to include ancillary metadata which can be useful for the interpretation of comparisons between (MAX)DOAS and satellite or model data, like averaging kernels, cloud conditions, location (latitude, longitude) of the effective air masses, etc, in addition to the trace gas or aerosol data. More general information about the GEOMS guidelines can be found at http://avdc.gsfc.nasa.gov/PDF/GEOMS/geoms-1.0.pdf. Use of the GEOMS format also ensures compliance to the ESA Atmospheric Validation Data Centre (EVDC, https://evdc.esa.int/) requirements which is important for data submitted for satellite validation.

With respect to reporting of spectra, a simple ASCII file format was developed during the FRM_4DOAS project for exchange of spectra. This will be developed into a netCDF format as part of the system development activities in FRM_4DOAS and a detailed description will be provided on the FRM_4DOAS web page. It is expected that this format will become the standard for MAXDOAS spectra reporting in the future.

The ASCII format is a simple 2 column format for wavelength and intensity. Each file has a header with lines starting with a hash sign (#) providing information on the measurement location, instrument, number of spectral points and number of spectra contained in the file. The header is followed by all the measurements of the day, each of which has a gain a header providing information on measurement mode, time, angles and integration time. These header lines do not start with a special character. An example of the first lines of such are file, here as example the Bremen UV observations during CINDI-2, are given below:

```
# Station = Cabauw (51.97 N,4.93 E)
# Institute = IUPB
# PI name = Andreas Richter (richter@iup.physik.uni-bremen.de)
# Instrument = UV
# Size of the detector = 1340
# Total number of records = 536
Date (DD/MM/YYYY) = 12/09/2016
UTC Time (hh:mm:ss) = 05:05:29.690
UTC Start Time (hh:mm:ss) = 05:04:57.270
UTC End Time (hh:mm:ss) = 05:06:02.120
Viewing Elevation Angle (deg) = 90.000
Viewing Azimuth Angle (deg) =   0.000
Measurement Type (OFFAXIS/DIRECT SUN/ALMUCANTAR/ZENITH/HORIZON) = ZENITH
Total Measurement Time (sec) =  64.850
Total Acquisition Time (sec) =  64.000
Exposure time (sec) =  12.800
Solar Zenith Angle (deg) =  91.602
Solar Azimuth Angle (deg) =  81.418 (North=0, East=90)
305.508000  3.743990660E+00
305.571844  3.743990660E+00
305.635688  3.743990660E+00
305.699531  3.743990660E+00
305.763373  3.743990660E+00
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