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

FRM4DOAS

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1 Introduction

In the next decade, the ESA Sentinel missions (S5-P, S4, and S5) will provide near-real-time (NRT) measurements of air quality trace gas products at high spatial and temporal resolution in support of the Copernicus Atmospheric Monitoring Service (CAMS). To ensure that the data products delivered by the atmospheric Sentinels match user requirements in terms of accuracy, precision and fitness for purpose, it is essential to establish a strong validation programme relying on well-established reference observational networks and related expert scientists.

Among the possible techniques, the Multi-Axis Differential Optical Absorption Spectroscopy (MAX-DOAS) provides ground-based reference data for most of the trace gas products targeted by the atmospheric Sentinels, i.e. nitrogen dioxide (NO_2), formaldehyde (HCHO), sulfur dioxide (SO_2), ozone (O_3), glyoxal (CHOCHO), etc. Moreover, MAX-DOAS measurements also deliver information on the vertical distribution of these trace gases as well as complementary information on aerosol extinction, which can be used for advanced validation studies. Currently, MAX-DOAS observations are being conducted by a number of research groups in various places of the World, however, no coordination has been attempted so far to harmonize and standardize these measurements in a traceable network configuration.

Considering the large variety of instrumental systems designed and operated by the MAX-DOAS research community, a necessary first step towards harmonization is to intercalibrate the different instruments and assess their mutual consistency and performance. As part of the Sentinel-5 Precursor (S5-P) validation programme and seven years after the first CINDI intercomparison, it has therefore been decided to organise a Second Cabauw Intercomparison campaign for Nitrogen Dioxide measuring Instruments (CINDI-2) with the target to intercompare and characterise a new and expanded generation of ground-based remote-sensing and in-situ air quality instruments intended for use in satellite validation. Like CINDI-1, CINDI-2 will benefit from the infrastructure developed by KNMI at the Cabauw Experimental Site for Atmospheric Research (CESAR; 51.971°N, 4.927° E; 0.7m below sea level) in the Netherlands. It will take place during one full month between 25 August and 7 October 2016.

The CINDI-2 campaign is highly complementary to the FRM_4DOAS project. It will provide an assessment of the current MAXDOAS instrument network capacity and will allow to evaluate the potential of the central processing system developed in FRM4DOAS to arrive at Fiducial Reference Measurements (FRM) for Air-Quality.

This document reviews the major requirements for a CINDI-2 campaign and the approach adopted to match them. We closely follow the reasoning developed by ESA in the "Requirements for the Geophysical Validation of Sentinel-5 Precursor Products Document" [RD-1].

2 CINDI-2 Campaign Requirements

R-1: In order to maximize its impact on the harmonisation of the current MAX-DOAS network, the CINDI-2 campaign should involve a sufficiently large number of MAX-DOAS groups operating different types of instruments (research grade/commercial; 1D-/2D-sytems). For the global validation of S5-P, it is also important that the participating MAX-DOAS instruments are routinely operated in a large variety of sites (e.g. polluted/unpolluted, high-altitude remote, marine, biomass burning) all around the World.

Approach adopted:

An invitation for participating to the CINDI-2 campaign was sent in January 2016 (i.e. 8 months before the start of the campaign) to the whole MAX-DOAS community. 26 different groups from 17 countries responded positively, which represents a total of 36 instruments regularly operated all over the World. It should be noted that about two third of these groups were not involved in the first CINDI campaign in 2009, indicating that the MAX-DOAS community has been growing significantly over the last 7 years. Among the participating instruments, 19 will be two-dimensional (2D) MAX-DOAS systems allowing for scans in both elevation and azimuth, 15 will be one-dimensional (1D) MAX-DOAS systems performing elevation scans in one fixed azimuthal direction, and the last 2 instruments will be simple zenith-sky DOAS systems. In comparison, only 3 bi-dimensional systems were operated during CINDI-1 which also demonstrates an evolution in the complexity (and potential) of the global MAXDOAS network. Importantly, the growing Pandonia FRM network developed under ESA/NASA funding will be represented during CINDI-2 (with 6 instruments) allowing for a complete assessment of the performance of all types of systems.

R-2: The consistency of the slant column abundances of key S5-P trace gases (NO_2, HCHO, O_3) measured by the different MAX-DOAS instruments participating to CINDI-2 should be assessed. Such an assessment will contribute to evaluating the current status of the MAX-DOAS network in terms of data quality and is the first step towards an improved network harmonisation.

Approach adopted:

The consistency between the trace gas slant column abundances measured by the different groups will be evaluated for all observational geometries (zenith, off-axis and direct-sun) through a two-week semi-blind intercomparison exercise, with a possible one-week extension in case of bad weather. The principle of such semi-blind exercise is that (1) all groups apply the same pre-defined data acquisition scheme and spectral analysis settings, and (2) trace gas slant column densities will be collected and intercompared on a daily basis under the coordination of an independent campaign referee. The strict application of a common data acquisition scheme (common pointing direction, same number and values of elevation and azimuth angles, synchronised data acquisition, etc) is essential to ensure that all instruments are probing the same air masses, and therefore to minimize the impact of the spatial and temporal variation of the trace gases (this is especially the case for NO_2) on the comparison results. For a proper testing of the consistency between the different MAX-DOAS systems, common spectral analysis settings will be used for all main campaign products, which will be NO_2, O_4, and O_3 in both the UV and visible ranges, and HCHO. The definition of the DOAS settings (wavelength ranges, cross-sections, etc) and data acquisition scheme will be based on results from the previous CINDI-1 and MAD-CAT intercomparison campaigns held in 2009 in Cabauw and in 2013 in Mainz, respectively, and on

MAXDOAS harmonisation efforts carried out within the framework of the EC FP7 projects NORS and QA4ECV.

The technical specifications and performance of each instrument (e.g. field of view, pointing accuracy, detector performance, etc) will be collected in advance of the campaign. This information will be useful for the interpretation of the measurements. During the two-week period before the formal semi-blind exercise (the so-called installation and warm-up phases), all the participating teams will be invited to perform specific calibration tests and to update their instrument fiche according to their calibration results, if necessary. The calibration tests, together with the data acquisition scheme and DOAS settings will be described in the 'Semi-blind Intercomparison Protocol' document.

R-3: The performance of the different trace gas and aerosol profiling tools available within the CINDI-2 consortium should be evaluated based on the slant column abundances measured during the semi-blind intercomparison exercise. Retrieving realistic profile shapes is important to verify inputs and assumptions used in the S5P air mass factor calculations, and to make the link between surface concentrations and column abundances in different atmospheric conditions (polluted/unpolluted, remote, etc).

Approach adopted:

A CINDI-2 Profiling Task Team (CPTT) will be created in advance of the campaign. The purpose of the CPTT will be to compare the different MAX-DOAS profiling tools available among the CINDI-2 consortium and to assess their consistency for retrieving aerosol extinction and trace gas concentration vertical profiles. The main tasks will be: (1) to make the inventory of the inversion tools/algorithms available within CINDI-2, including for each of them a short description of the retrieval method used, (2) to agree on the comparison tests to be performed and on the corresponding common settings (e.g. a priori profiles, altitude grid, pressure and temperature profiles, etc) and output data format to be used by all groups, and (3) to coordinate first comparison tests during the campaign. Days with favorable meteorological conditions will be selected for initial processing of target species of relevance for S5P validation (i.e. NO_2, HCHO, and aerosols).

If possible, preliminary comparison results will be shown during the campaign. As verification purpose, the retrieved quantities (vertical profiles, surface concentrations, and vertical column densities) will be compared to measurements from the ancillary instruments that will be simultaneously operated during the campaign. In particular NO_2 sondes and lidar, long-path DOAS, sunphotometer (AOD), near-surface concentrations from in-situ monitors, etc will be used for this purpose. This validation using independent data is important for assessing the MAX-DOAS network as a reference network for ground-truthing of current and future satellite missions. The CINDI-2 profiling activities will be formally extended as part of the Round-Robin exercise of profiling tools to be carried out in the FRM_4DOAS project.

R-4: As for all remote sensing techniques, MAX-DOAS observations average over space and time, providing integrated values representative of a certain air volume. This volume being similar to the spatial domain that will be probed by TROPOMI/S5-P and the future Sentinel 4 and 5 (i.e. approx. 7x7 km^2), MAX-DOAS observations are well suited for the validation of trace gas measurements by these satellite experiments. To investigate the range of validity of this

statement, the impact of local gradients on MAX-DOAS measurements at the scale of the satellite ground-pixel should be investigated during CINDI-2.

Approach adopted:

CINDI-2 will be a unique opportunity to investigate and characterize the horizontal representativeness of MAX-DOAS trace gas and aerosol observations since about 17 2D-MAX-DOAS systems, i.e. scanning the atmosphere in both elevation and azimuth directions, will operate in parallel. A specific data acquisition scheme for these 2D-instruments will be prepared, combining a selection of different azimuth viewing directions covering the 0-360° azimuth range. O_4 measurements will be used to determine the azimuth-dependent horizontal extent of these MAXDOAS observations. The horizontal distribution of the trace gas column and concentrations will be assessed through comparison with mobile measurements that will be regularly performed around Cabauw during the most intensive part of the campaign.

R-5: The standard error budget on MAX-DOAS measurements should be assessed, based on the CINDI-2 campaign results.

Approach adopted:

The level of agreement between the trace gas slant column abundances retrieved by the different groups during the semi-blind exercise will be used to revise the current standard error budget associated to MAX-DOAS measurements. In addition, the uncertainties related to more advanced products like vertical profiles, surface concentrations, and vertical column densities will be assessed, based on the profile comparison results.

3 References

[RD-1]: Requirements for the Geophysical Validation of Sentinel-5 Precursor Products document (ref. S5P-RS-ESA-SY-164).

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