THE NDACC MAX-DOAS CENTRAL PROCESSING SERVICE IN SUPPORT TO AIR QUALITY SATELLITE SENSORS VALIDATION

F. Hendrick[1], M. M. Friedrich[1], C. Fayt[1], S. Beirle[2], U. Frieß[3], A. Richter[4], T. Bösch[4], K. Kreher[5], A. Piters[6], T. Wagner[2], A. Bais[7], D. Karagkiozidis[7], M. Yela González[8], M. Navarro Comas[8], O. Puentedura Rodríguez[8], J.-L. Tirpitz[3], A. Dehn[9], P. Castracane[9], S. Casadio[9], and M. Van Roozendael[1]

[1]IASB-BIRA, Brussels, Belgium (francois.hendrick@aeronomie.be); [2]Max-Planck Institute for Chemistry, Mainz, Germany; [3]Institute for Environmental Physics, University of Heidelberg, Heidelberg, Germany; [4]Institute for Environmental Physics, University of Bremen, Bremen, Germany; [5]BK Scientific GmbH, Mainz, Germany; [6]Royal Netherlands Meteorological Institute (KNMI), De Bilt, The Netherlands; [7]Aristole University of Thessaloniki, Thessaloniki, Greece; [8]Instituto Nacional de Técnica Aeroespacial (INTA), Madrid, Spain; [9]ESA-ESRIN, Frascati, Italy

https://frm4doas.aeronomie.be

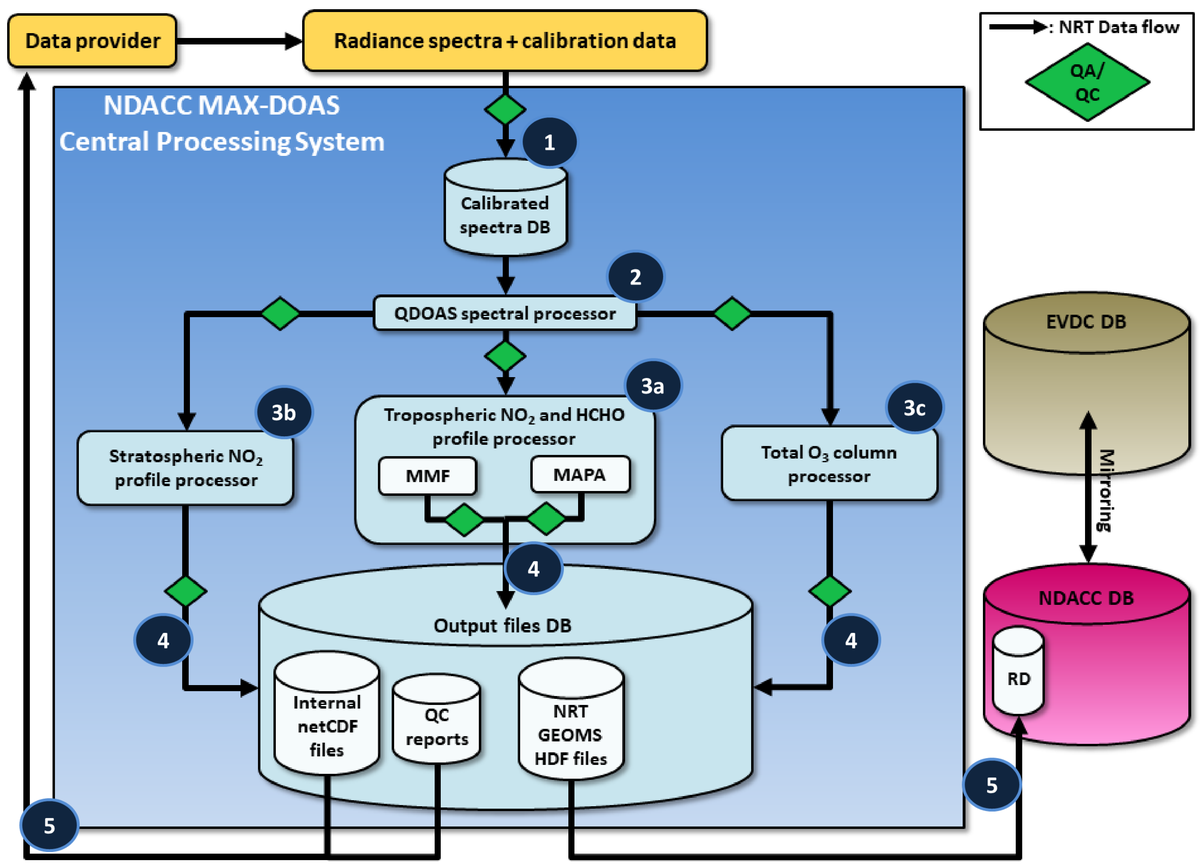
I. SUMMARY

In order to ensure that products delivered by air quality satellite sensors meet user requirements in terms of accuracy, precision and fitness for purpose, it is essential to develop a robust validation strategy relying on well-established and traceable reference measurements. In this context, the ESA Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations (FRM$_4$DOAS) activity is aiming at further harmonizing Multi-Axis Differential Optical Absorption Spectroscopy (MAX-DOAS) measurements. Since it provides vertically-resolved information on atmospheric gases at a horizontal scale approaching the one from nadir backscatter satellite sensors, the ground-based MAX-DOAS technique has been recognized as a valuable source of correlative data for validating space-borne observations of atmospheric species such as NO_2, HCHO, SO_2, O_3, etc.

Here we present the main aspects and status of the first near-real-time (24h latency) central processing service for MAX-DOAS instruments that has been developed in the framework of the FRM$_4$DOAS activity and which is operated as part of the Network for the Detection of Atmospheric Composition Change (NDACC). Since November 2020, the processing system, which includes state-of-the-art retrieval algorithms, delivers on a daily basis tropospheric NO_2 vertical profile and total O_3 column data from about 15 stations to the NDACC Rapid Delivery and ESA Validation Data Centre (EVDC) databases.

The NDACC MAX-DOAS central processing service and its future upscaling in terms of stations and data products will ensure that MAX-DOAS observations at a FRM quality level will be made available for the validation of present and future satellite missions like the Copernicus atmospheric Sentinels (5p, 4, 5).

II. MAX-DOAS CENTRAL PROCESSING SYSTEM



Main processing steps:

1. Uploading of level-1 files (spectrally calibrated radiance spectra) on a dedicated incoming FTP server by instrument PIs and storage of the files on a dedicated database
2. DOAS analysis using the QDOAS spectral fitting software (Fayt et al., 2011)
3. Level-2 data product retrievals using the following algorithms:
   - 3a Parameterisation-based MAPA (Beirle et al., 2019) and Optimal-Estimation-based MMF (Friedrich et al., 2019) for lower tropospheric profiles and vertical columns of NO_2, HCHO, and aerosols (see also Frieß et al., 2019)
   - 3b BIRA-IASB Optimal-Estimation-based profiling tool for stratospheric NO_2 vertical profiles (Hendrick et al., 2004)
   - 3c Standard AMF-based NDACC approach for the total O_3 column retrieval (Hendrick et al., 2011)
4. Generation of level-2 data files: (1) internal netCDF files that contain the complete and fully traceable set of retrieval variables and ancillary data, and (2) standard GEOMS HDF4 files
5. Automatic submission of the GEOMS HDF4 files to the NDACC Rapid Delivery repository with mirroring on the EVDC database + delivery of netCDF files to instrument PIs

QA/QC procedures:

- QA/QC tests on the retrieved results after each processing step + various diagnostic checks allowing the detection of anomalies throughout the processing chain
- Generation of reports (status of processed files, statistics, list of eventual anomalies, etc); In the case of anomalies, e-mail alerts are sent to the service administrators and concerned instrument PIs.

Data policy:

- Creative Commons (CC) license system

Data traceability:

- DOI assignment to each data set

III. NDACC MAX-DOAS SERVICE READINESS (11/2021)

Products maturity:

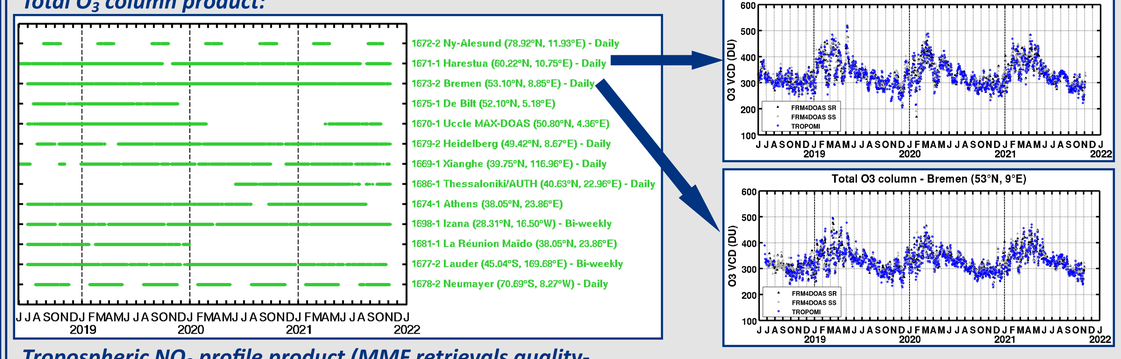
Extensive verification and validation exercises have shown that:

- Total O_3 column and tropospheric NO_2 vertical profile products are mature enough for submission on NDACC/RD and EVDC DBs
- Stratospheric NO_2 and tropospheric HCHO vertical profile products need to be further consolidated and therefore are currently not submitted on NDACC/RD and EVDC DBs

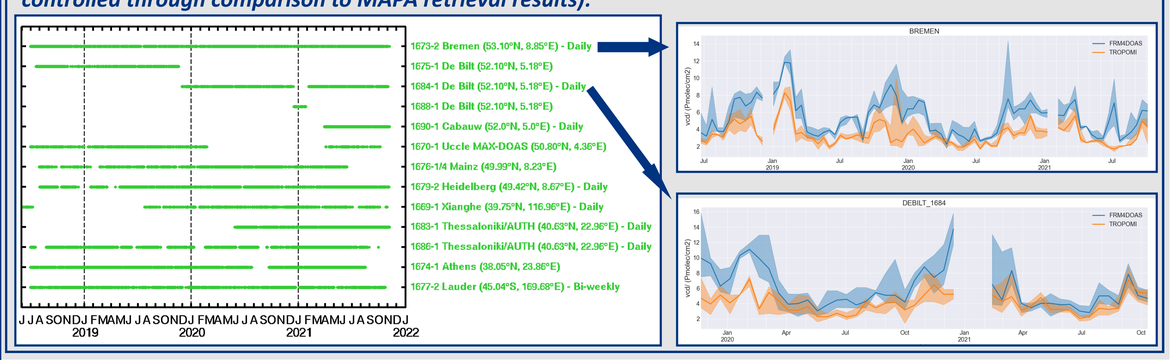
For further details, see https://frm4doas.aeronomie.be/ProjectDir/Deliverables/FRM4DOAS_CCN02_D21_Operational_Processing_System_and_Test_Report_document_v1.0_20200623.pdf

Data sets available on NDACC/RD and EVDC databases:

Total O_3 column product:



Tropospheric NO_2 profile product (MMF retrievals quality-controlled through comparison to MAPA retrieval results):



IV. FUTURE SERVICE DEVELOPMENTS

New/consolidated MAX-DOAS products foreseen as part of the new FRM$_4$DOAS-2.0 R&D project (09/2021-08/2025):

- Consolidated stratospheric NO_2 profile product
- NRT cloud product
- Consolidated aerosol product
- Urban tropospheric NO_2 product

V. REFERENCES

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VI. ACKNOWLEDGEMENTS

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