FRM_4DOAS CCN02 overview

F. Hendrick and FRM_4DOAS partners

FRM$_4$DOAS Team

BELGISCH INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT D'AERONOMIE SPATIALE DE BELGIQUE BELGIAN INSTITUTE OF SPACE AERONOMY BELGISCH INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT D'AERONOMIE SPATIALE DE BELGIQUE BELGIAN INSTITUTE OF SPACE AERONOMY BELGISCH INSTITUUT VOOR RUIMTE-AERONOMIE INSTITUT D'AERO

- **BIRA-IASB (Lead):** M. Van Roozendael, F. Hendrick, C. Fayt, M. Friedrich
- **IUP-Bremen:** A. Richter, T. Bösch
- **IUP-Heidelberg:** U. Friess, L. Tirpitz
- **MPIC:** T. Wagner, S. Beirle, Y. Wang, S. Dörner
- **KNMI:** A. Piters
- **BK Scientific:** K. Kreher
- **AUTH:** A. Bais, D. Karagkiozidis
- **INTA:** M. Navarro Comas, C. Prados Roman, O. Puentedura, M. Yela

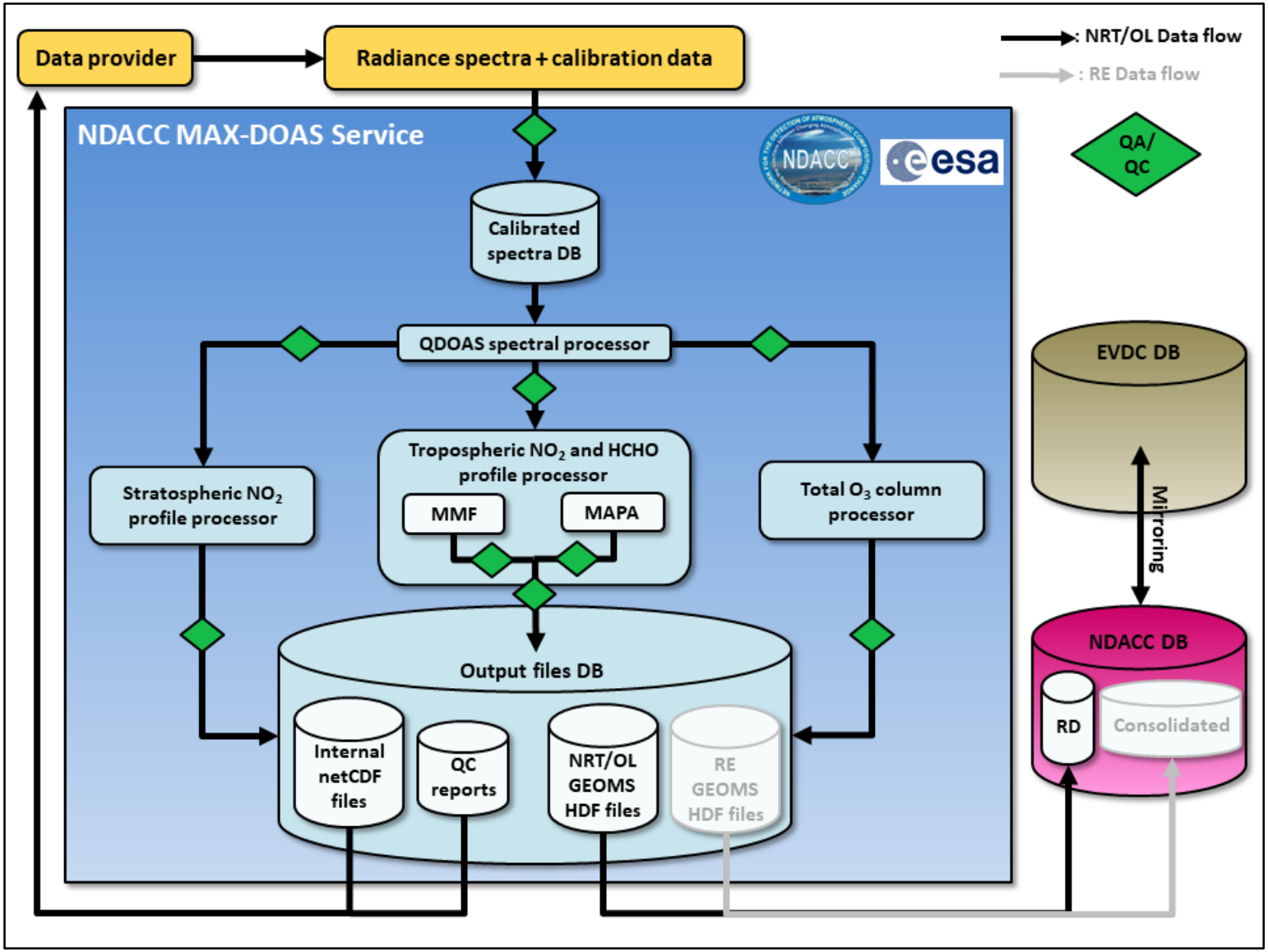
WP1500: NDACC MAX-DOAS Service Kick-off

To create the framework and to develop the operational code needed for a kick-off of the NDACC MAX-DOAS Service, in view of the future Service upscaling expected in the Copernicus follow-up project.

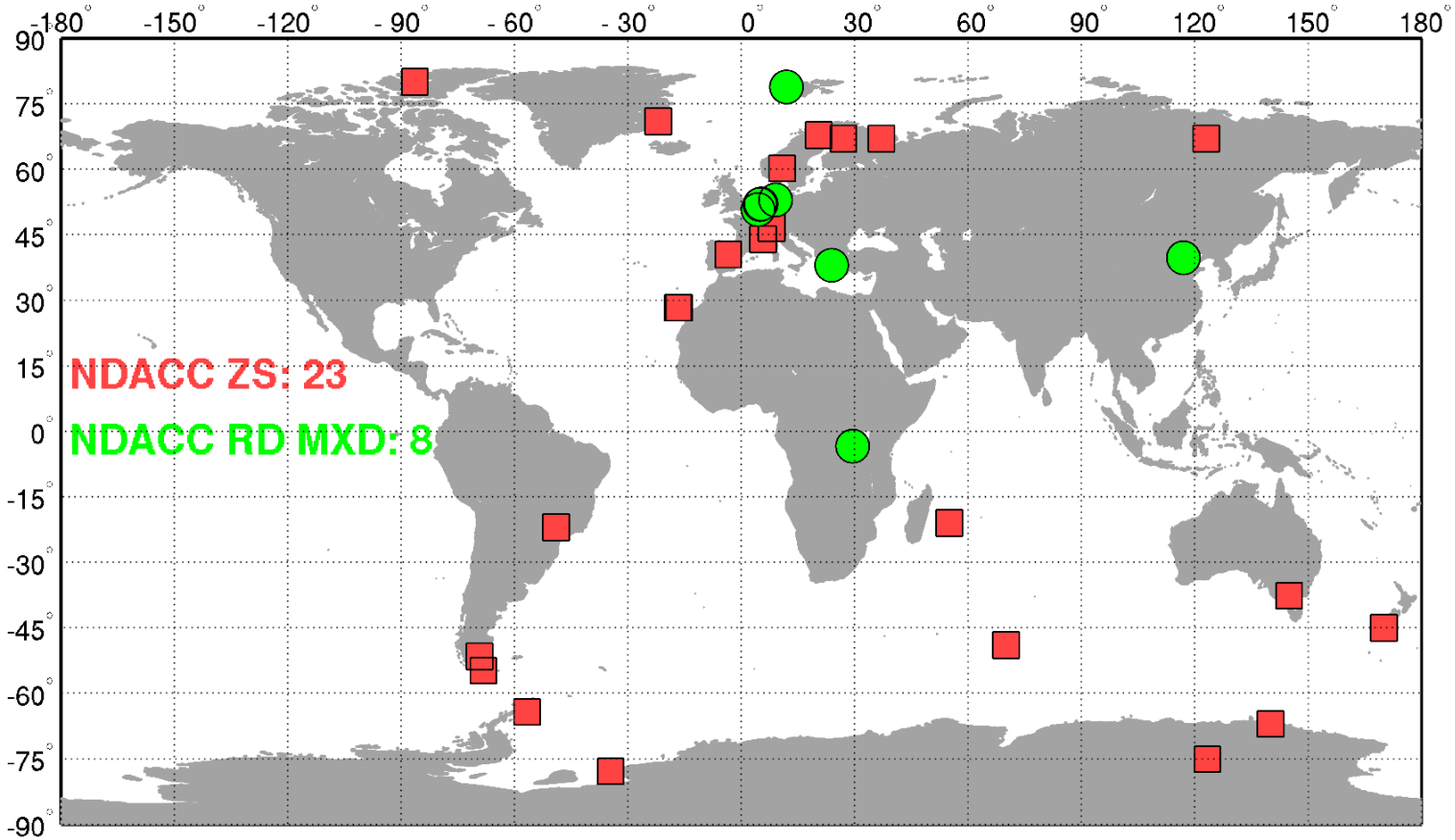
Service concept elements:

- Products: tropospheric NO_2 and HCHO vertical profiles, total O_3 columns, and stratospheric NO_2 vertical profiles
- Sites: a limited selection (~5-10) of (NDACC-certified) instruments
- Focus on NRT processing (24h latency)
- Integration in NDACC/EVDC through the establishment of:
  - Data stream between the FRM_4DOAS Operational Central Processing System and the NDACC and EVDC databases
  - MAX-DOAS NDACC instrument and data analysis certification procedures

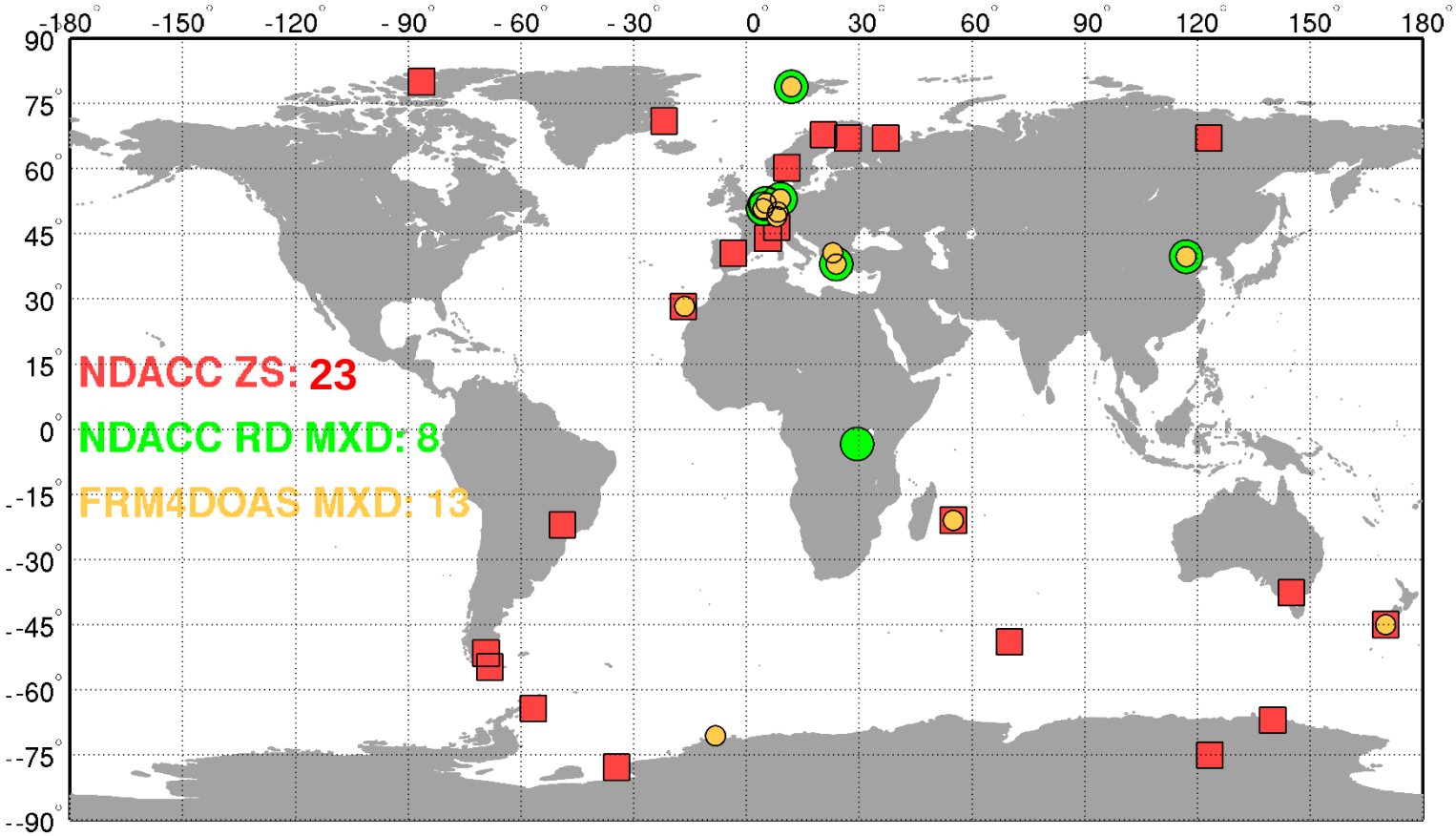
NDACC MAX-DOAS Service



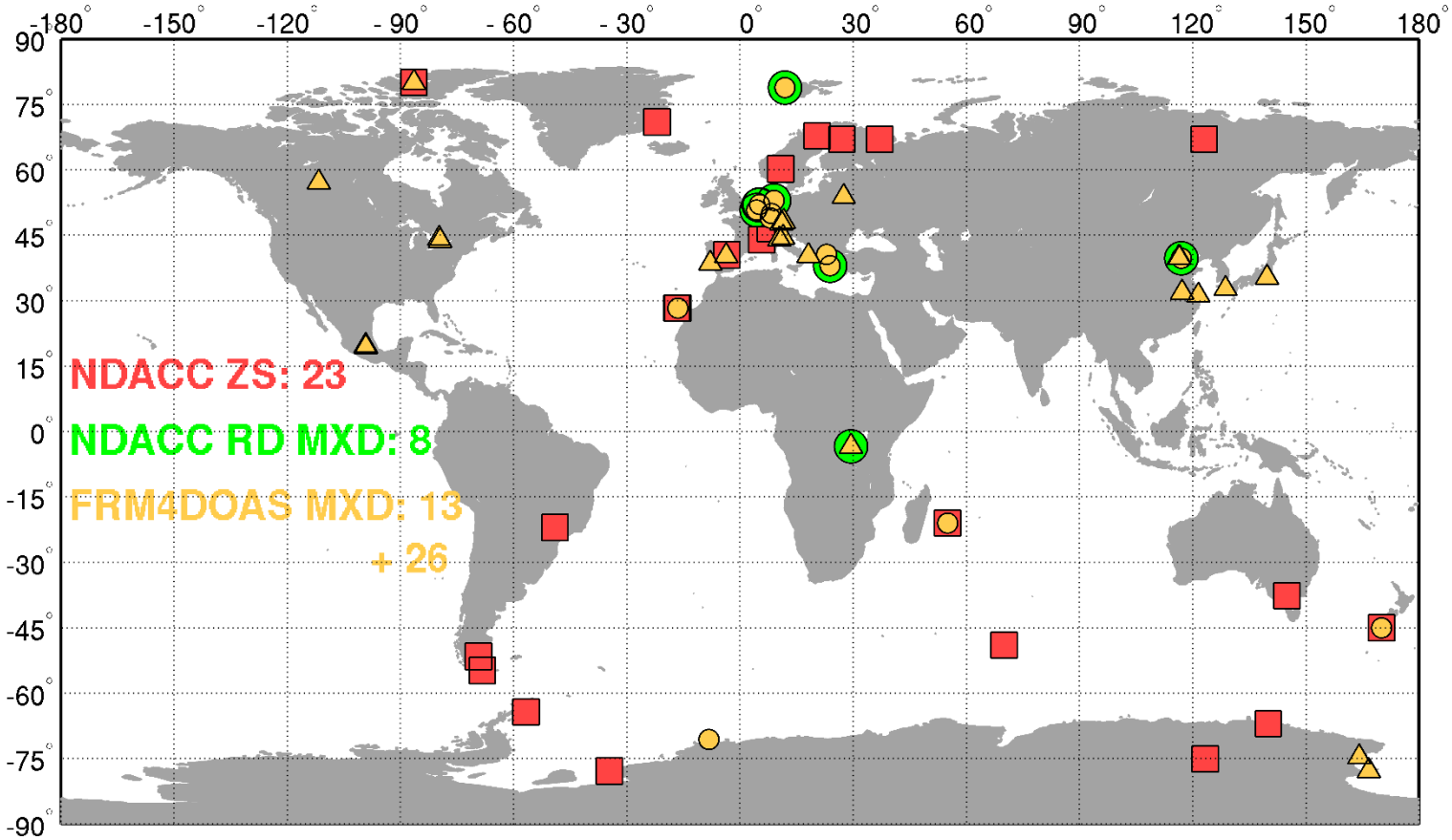
MAX-DOAS stations in NDACC



MAX-DOAS stations in NDACC



MAX-DOAS stations in NDACC



WP1500 structure

WP1500:
NDACC MAX-DOAS Service Kick-off

WP1510:
Algorithmic Optimisation

Optimisation of the trace gas vertical profiling processors in terms of retrieval results accuracy and computing performance

WP1500 structure

WP1500:
NDACC MAX-DOAS Service Kick-off

WP1510:
Algorithmic Optimisation

WP1520:
CPS Operationalisation

WP1500 structure

WP1500:
NDACC MAX-DOAS Service Kick-off

WP1510:
Algorithmic Optimisation

WP1520:
CPS Operationalisation

- To make the CPS code operational within NDACC/EVDC:
  - *To run the operational code in NRT mode (latency time<24h) on a selection of (NDACC-certified) MAX-DOAS instruments*
  - *Operational data stream between FRM4DOAS and NDACC and EVDC DB*
- To create the framework for future service upscaling (certification procedures, user data policy, and datasets DOI)

WP1500 structure

WP1500:
NDACC MAX-DOAS Service Kick-off

WP1510:
Algorithmic Optimisation

WP1520:
CPS Operationalisation

WP1530:
CPS Verification and Validation

Verification and validation of the Operational CPS code, retrieval results, and system performance

WP1510: Algorithmic Optimisation

Tasks:

- **To improve the QC flagging in MMF and MAPA and their consistency**
  - Consistence check on VCD (within errors)
  - Crude profile consistence check (percentage)
  - One code not "error", so at least only "warning"
  - Extra dscd error (extra error < 3 x QDOAS dscd error)

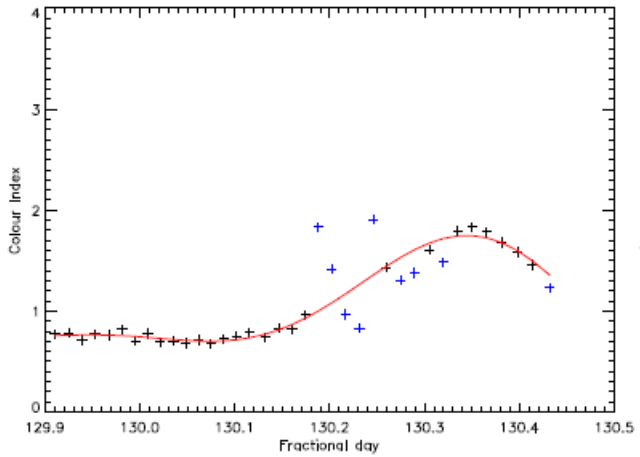
WP1510: Algorithmic Optimisation

Tasks:

- **To improve the QC flagging in MMF and MAPA and their consistency**
  - Consistence check on VCD (within errors)
  - Crude profile consistence check (percentage)
  - One code not "error", so at least only "warning"
  - Extra dscd error (extra error < 3 x QDOAS dscd error)

M. Friedrich talk ~9h40

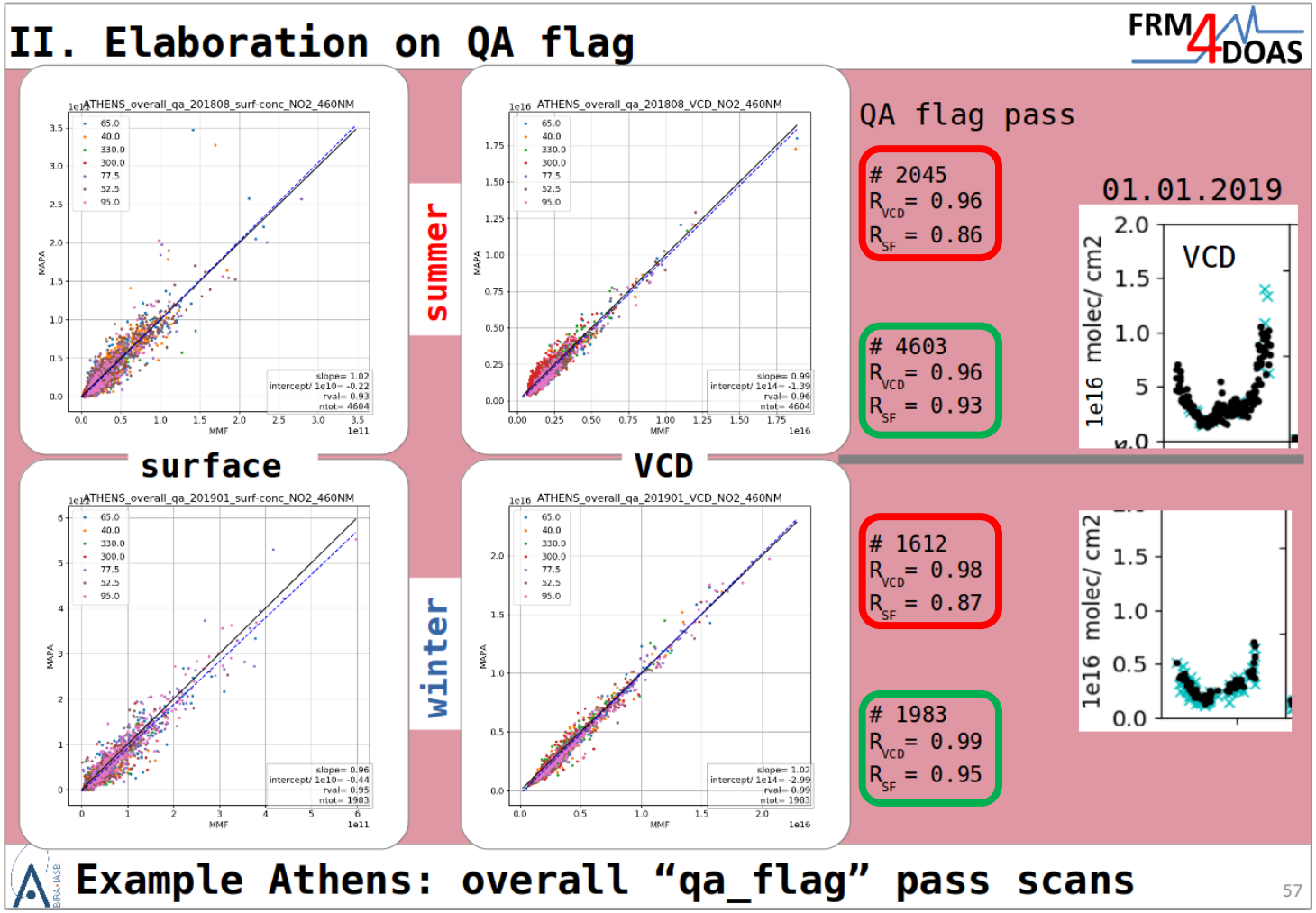
+ Broken-cloud flagging:



WP1510: Algorithmic Optimisation

Tasks:

- To improve the QC flagging in MMF and MAPA and their consistency



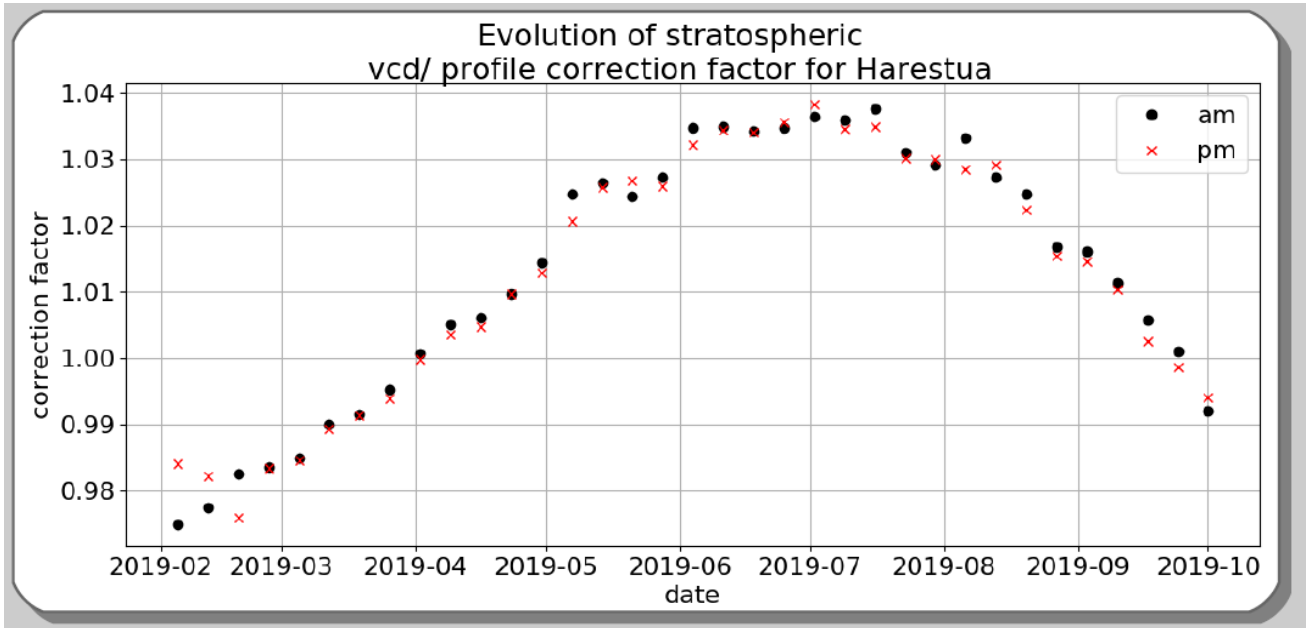
M. Friedrich talk ~9h40

WP1510: Algorithmic Optimisation

Tasks:

- To improve the QC flagging in MMF and MAPA and their consistency

- **Correction for the temperature dependence of the NO_2 cross sections in the stratospheric NO_2 profiling algorithm**



(T profile climatology produced by MPIC with ECMWF data)

WP1510: Algorithmic Optimisation

Tasks:

- To improve the QC flagging in MMF and MAPA and their consistency
- Correction for the temperature dependence of the NO_2 cross sections in the stratospheric NO_2 profiling algorithm
- **Set-up of QA/QC flagging for stratospheric products**

M. Friedrich talk ~9h40

WP1520: CPS Operationalisation

Tasks – Part 1 (technical):

- To review and improve/optimise all system programs (structure, content, input/output data, settings, config, and log files)
  - *Clean code with high level of modularity (-> service upscaling)*

WP1520: CPS Operationalisation

Tasks – Part 1 (technical):

- To review and improve/optimise all system programs (structure, content, input/output data, settings, config, and log files)
  - *Clean code with high level of modularity (-> service upscaling)*

- To create the framework and scripts for running the CPS on HPC
  - *150 spectra files in Xianghe: 1h HPC ↔ 12.5 h compute servers*

M. Friedrich
talk ~9h40

WP1520: CPS Operationalisation

Tasks – Part 1 (technical):

- To review and improve/optimise all system programs (structure, content, input/output data, settings, config, and log files)
  - *Clean code with high level of modularity (-> service upscaling)*
- To create the framework and scripts for running the CPS on HPC
  - *150 spectra files in Xianghe: 1h HPC ↔ 12.5 h compute servers*
- To establish a working data stream between the FRM_4DOAS Central Processing System and the NDACC and EVDC databases

Data stream to NDACC and EVDC

NDACC database ready to ingest GEOMS files produced by the Service

PI_NAME	PI_EMAIL	DATA_LOCATION	DATA_SOURCE	NDACC affiliation status	NDACC RD status
Van Roozendael;Michel	michelv@aeronomie.be	XIANGHE	UVVIS.DOAS.OFFAXIS.NO2_BIRA.IASB007_FRM4DOAS.01	No	Yes
			UVVIS.DOAS.OFFAXIS.H2CO_BIRA.IASB007_FRM4DOAS.01	No	Yes
			UVVIS.DOAS.ZENITH.NO2_BIRA.IASB007_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.O3_BIRA.IASB007_FRM4DOAS.01	No	No
		UCCLE	UVVIS.DOAS.OFFAXIS.NO2_BIRA.IASB011_FRM4DOAS.01	No	Yes
			UVVIS.DOAS.OFFAXIS.H2CO_BIRA.IASB011_FRM4DOAS.01	No	Yes
			UVVIS.DOAS.ZENITH.NO2_BIRA.IASB011_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.O3_BIRA.IASB011_FRM4DOAS.01	No	No
		HARESTUA	UVVIS.DOAS.ZENITH.NO2_BIRA.IASB004_FRM4DOAS.01	Ye	
			UVVIS.DOAS.ZENITH.O3_BIRA.IASB004_FRM4DOAS.01	Ye	
		LA.REUNION.MAIDO	UVVIS.DOAS.OFFAXIS.NO2_BIRA.IASB009_FRM4DOAS.01	No	
			UVVIS.DOAS.OFFAXIS.H2CO_BIRA.IASB009_FRM4DOAS.01	No	
			UVVIS.DOAS.ZENITH.NO2_BIRA.IASB009_FRM4DOAS.01	No	
			UVVIS.DOAS.ZENITH.O3_BIRA.IASB009_FRM4DOAS.01	No	
Burrows;John P.	burrows@iup.physik.uni-bremen.de	NY.ALESUND	UVVIS.DOAS.OFFAXIS.NO2_IUP003_FRM4DOAS.01	No	
			UVVIS.DOAS.OFFAXIS.H2CO_IUP003_FRM4DOAS.01	No	
			UVVIS.DOAS.ZENITH.NO2_IUP003_FRM4DOAS.01	Ye	
			UVVIS.DOAS.ZENITH.O3_IUP003_FRM4DOAS.01	Ye	
		BREMEN	UVVIS.DOAS.OFFAXIS.NO2_IUP002_FRM4DOAS.01	No	
			UVVIS.DOAS.OFFAXIS.H2CO_IUP002_FRM4DOAS.01	No	
			UVVIS.DOAS.ZENITH.NO2_IUP002_FRM4DOAS.01	No	
			UVVIS.DOAS.ZENITH.O3_IUP002_FRM4DOAS.01	No	
		ATHENS	UVVIS.DOAS.OFFAXIS.NO2_IUP008_FRM4DOAS.01	No	
			UVVIS.DOAS.OFFAXIS.H2CO_IUP008_FRM4DOAS.01	No	
			UVVIS.DOAS.ZENITH.NO2_IUP008_FRM4DOAS.01	No	
			UVVIS.DOAS.ZENITH.O3_IUP008_FRM4DOAS.01	No	
Piters;Ankie	ankie.piters@knmi.nl	DE.BILT	UVVIS.DOAS.OFFAXIS.NO2_KNMI004_FRM4DOAS.01	No	
			UVVIS.DOAS.ZENITH.NO2_KNMI004_FRM4DOAS.01	No	
			UVVIS.DOAS.ZENITH.O3_KNMI004_FRM4DOAS.01	No	
Wagner;Thomas	thomas.wagner@mpic.de	MAINZ	UVVIS.DOAS.OFFAXIS.NO2_MPIC001_FRM4DOAS.01	No	
			UVVIS.DOAS.OFFAXIS.H2CO_MPIC001_FRM4DOAS.01	No	
			UVVIS.DOAS.ZENITH.NO2_MPIC001_FRM4DOAS.01	No	
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			UVVIS.DOAS.OFFAXIS.H2CO_MPIC002_FRM4DOAS.01	No	
			UVVIS.DOAS.ZENITH.NO2_MPIC002_FRM4DOAS.01	No	No
			UVVIS.DOAS.OFFAXIS.NO2_MPIC003_FRM4DOAS.01	No	No
			UVVIS.DOAS.OFFAXIS.H2CO_MPIC003_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.NO2_MPIC003_FRM4DOAS.01	No	No
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			UVVIS.DOAS.OFFAXIS.H2CO_MPIC004_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.NO2_MPIC004_FRM4DOAS.01	No	No
Friess;Udo	udo.friess@iup.uni-heidelberg.de	NEUMAYER	UVVIS.DOAS.OFFAXIS.NO2_UHEIDELBERG002_FRM4DOAS.01	No	No
			UVVIS.DOAS.OFFAXIS.H2CO_ UHEIDELBERG002_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.NO2_UHEIDELBERG002_FRM4DOAS.01	Yes	No
			UVVIS.DOAS.ZENITH.O3_UHEIDELBERG002_FRM4DOAS.01	Yes	No
		HEIDELBERG	UVVIS.DOAS.OFFAXIS.NO2_UHEIDELBERG001_FRM4DOAS.01	No	No
			UVVIS.DOAS.OFFAXIS.H2CO_ UHEIDELBERG001_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.NO2_UHEIDELBERG001_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.O3_UHEIDELBERG001_FRM4DOAS.01	No	No
Querel;Richard	Richard.Querel@niwa.co.nz	LAUDER	UVVIS.DOAS.OFFAXIS.NO2_NIWA007_FRM4DOAS.01	No	No
			UVVIS.DOAS.OFFAXIS.H2CO_NIWA007_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.NO2_NIWA007_FRM4DOAS.01	Yes	No
			UVVIS.DOAS.ZENITH.O3_NIWA007_FRM4DOAS.01	Yes	No
Bais;Alkis	abais@auth.gr	THESSALONIKI_AUTH	UVVIS.DOAS.OFFAXIS.NO2_AUTH007_FRM4DOAS.01	No	No
			UVVIS.DOAS.OFFAXIS.H2CO_AUTH007_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.NO2_AUTH007_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.O3_AUTH007_FRM4DOAS.01	No	No
		THESSALONIKI_CIRI	UVVIS.DOAS.OFFAXIS.NO2_AUTH008_FRM4DOAS.01	No	No
			UVVIS.DOAS.OFFAXIS.H2CO_AUTH008_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.NO2_AUTH008_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.O3_AUTH008_FRM4DOAS.01	No	No
Navarro;Monica	navarrocm@inta.es	IZANA	UVVIS.DOAS.OFFAXIS.NO2_INTA001_FRM4DOAS.01	No	No
			UVVIS.DOAS.ZENITH.NO2_INTA001_FRM4DOAS.01	Yes	Yes
			UVVIS.DOAS.ZENITH.O3_INTA001_FRM4DOAS.01	Yes	Yes

- **GEOMS files successfully tested against NDACC QA checkers**
- **Single submission to NDACC + mirroring by EVDC (green light from NILU/A. M. Fjaeraa)**

WP1520: CPS Operationalisation

Tasks – Part 2 (« administrative » framework):

- NDACC MAX-DOAS instrument and data retrieval certification procedures

NDACC affiliation and certification

New NDACC Appendix VII protocol (M. Van Roozendael/K. Kreher):

Appendix VII

Protocol for NDACC UV/Vis instrument operation and data analysis

October 2019

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. Data quality criteria are also provided for all zenith-sky and MAX-DOAS end products, i.e. vertical column abundances of stratospheric NO_2 and ozone, vertical profiles of stratospheric BrO and NO_2 as well as vertical profiles of tropospheric NO_2 and HCHO.

1

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 turns implies 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 (general 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 measurements, 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 an input (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 zenith-sky instruments, 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 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

NDACC affiliation and certification

1) **Official demand for affiliation needed for all MAX-DOAS instruments**

2) **Certification:**

- ***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 intercomp. 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 (e.g. Bremen instrument in Ny-Alesund)

WP1520: CPS Operationalisation

Tasks – Part 2 (« administrative » framework):

- NDACC MAX-DOAS instrument and data retrieval certification procedures (new NDACC Appendix VII Protocol)

- DOI and data policy and related procedures for NDACC MAX-DOAS Service products

DOI

- Granularity: one doi per group
- DOIs (+ landing page) assigned by NILU: e.g. IUP-Bremen stations DOI

https://doi.org/10.21336/apdw-nb87

evdc esa

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Updated: 20 Apr 2020

Universität Bremen

Institute of Environmental Physics, University of Bremen (IUP-UB), Bremen, Germany

Data download:

ftp://ftp.cpc.ncep.noaa.gov/ndacc/RD/bremen/hdf/uvvis/
ftp://ftp.cpc.ncep.noaa.gov/ndacc/RD/nyalesund/hdf/uvvis/
ftp://ftp.cpc.ncep.noaa.gov/ndacc/RD/athens/hdf/uvvis/

Title:

NDACC MAX-DOAS Service data sets from IUP-UB stations available at the NDACC and EVDC Data Handling Facilities

Authors:

John P. Burrows (instruments' PI), Institute of Environmental Physics (IUP-UB), University of Bremen, Bremen, Germany
Andreas Richter, Institute of Environmental Physics, University of Bremen (IUP-UB), Bremen, Germany
Folkard Wittrock, Institute of Environmental Physics, University of Bremen (IUP-UB), Bremen, Germany
Evangelos Gerasopoulos, National Observatory of Athens (NOA), Athens, Greece
Myrto Gratsea, National Observatory of Athens (NOA), Athens, Greece

Publication year:

2020

Subject:

Atmospheric Science

Keywords:

Network for the Detection of Atmospheric Composition Change
Fiducial Reference Measurements
Atmospheric trace gases
NO_2
HCHO
O_3
Differential Optical Absorption Spectroscopy
Remote Sensing
Ground-based instrumentation

Contact person:

Andreas Richter, IUP-UB (Andreas.Richter@iup.physik.uni-bremen.de)

Date of creation:

30/04/2020

Size:

Xy GB

Format:

GEOMS HDF

Language:

English

Rights:

Creative Commons License (see https://creativecommons.org/licenses/by-nc-sa/4.0/ for more information):

Station	Instrument	Affiliation	CC License
Ny-Ålesund	ZS-DOAS UV-vis Research grade/custom-built	IUP-UB	CC BY-NC-SA
Bremen	MAX-DOAS UV-vis Research grade/custom-built	IUP-UB	CC BY-NC-SA
Athens	MAX-DOAS UV-vis Research grade/custom-built	IUP-UB / NOA	CC BY-NC-SA

In addition to the CC license, the NDACC Data Use Agreement including publication co-authorship policy must always be respected (see http://www.ndaccdemo.org/data/use-agreement).

Resource type:

Dataset

Methods:

The present NDACC MAX-DOAS Service data sets are generated by the FRM4DOAS central processing facility (see http://frm4doas.aeronomie.be/index.php), which includes the following algorithms for the retrieval of the different Service products:

Lower tropospheric NO_2 and HCHO vertical profiles: TROPO algorithm based on the Optimal-Estimation-based Mexican Maxdoas Fit algorithm (MMF; Friedrich et al., 2019) using the parameterized MAinz Profile Algorithm (MAPA; Beirle et al., 2019) retrieval results as quality control.

Total O_3 column: NDACC twilight zenith-sky approach algorithm (Hendrick et al., 2011).

Stratospheric NO_2 vertical profile: Twilight zenith-sky Optimal-Estimation-based algorithm developed at BIRA (Hendrick et al., 2004).

Beirle, S., S. Dörner, S. Donner, J. Remmers, Y. Wang, and T. Wagner, The Mainz profile algorithm (MAPA), Atmos. Meas. Tech., 12, 1785–1806, https://doi.org/10.5194/amt-12-1785-2019, 2019.

Friedrich, M. M., C. Rivera, W. Stremme, Z. Ojeda, J. Arellano, A. Bezanilla, J. A. García-Reynoso, and M. Grutter, NO_2 vertical profiles and column densities from MAX-DOAS measurements in Mexico City, Atmos. Meas. Tech., 12, 2545–2565, https://doi.org/10.5194/amt-12-2545-2019, 2019.

Hendrick, F., J.-P. Pommereau, F. Goutail, R. D. Evans, D. Ionov, A. Pazmino, E. Kyrö, G. Held, P. Eriksen, V. Dorokhov, M. Gil, and M. Van Roozendael, NDACC/SAOZ UV-visible total ozone measurements: Improved retrieval and comparison with correlative ground-based and satellite observations, Atmos. Chem. Phys., 11, 5975–5995, https://doi.org/10.5194/acp-11-5975-2011, 2011.

Hendrick, F., B. Barret, M. Van Roozendael, H. Boesch, A. Butz, M. De Mazière, F. Goutail, C. Hermans, J.-C. Lambert, K. Pfeilsticker, and J.-P. Pommereau, Retrieval of nitrogen dioxide stratospheric profiles from ground-based zenith-sky UV-visible observations: Validation of the technique through correlative comparisons, Atmos. Chem. Phys., 4, 2091–2106, https://doi.org/10.5194/acp-4-2091-2004, 2004.

Versioning tables:

Ny-Ålesund:

Processor version	Date of issue	Algorithm versions		
		TROPO	O3TOTAL	NO2STRATO
FRM4DOAS.01	30/04/2020	N/A	01	01

NDACC data policy approach: Creative Commons license

Instrument number	Station name	Affiliation	CC license
1669	XIANGHE	BIRA-IASB	CC-BY-SA-4.0
1670	UCCLE	BIRA-IASB	CC-BY-SA-4.0
1671	HARESTUA	BIRA-IASB	CC-BY-SA-4.0
1681	LA.REUNION.MAIDO	BIRA-IASB	CC-BY-SA-4.0
1672	NY.ALESUND	IUP	CC-BY-NC-SA
1673	BREMEN	IUP	CC-BY-NC-SA
1674	ATHENS	IUP	CC-BY-NC-SA
1675/1684	DEBILT	KNMI	CC-BY-SA-4.0
1676	MAINZ	MPIC	CC-BY-NC-SA
1677	LAUDER	NIWA	CC-BY-SA-4.0
1678	NEUMAYER	UHEIDELBERG	CC-BY-NC-SA
1679	HEIDELBERG	UHEIDELBERG	CC-BY-NC-SA
1683	THESSALONIKI	AUTH	CC-BY-NC-SA
1698	IZANA	INTA	CC-BY-NC-SA

CC-By-SA (4.0) license: open – but credits required

CC-BY-NC-SA license: not open for commercial use

WP1520: CPS Operationalisation

Tasks – Part 2 (« administrative »):

- NDACC MAX-DOAS instrument and data retrieval certification procedures (new NDACC Appendix VII Protocol)

- DOI and data policy and related procedures for NDACC MAX-DOAS Service products

- Consultation of the UV/VIS DOAS community (questionnaire)

NDACC MAX-DOAS Service questionnaire

NDACC MAX-DOAS Service

Questionnaire for using the NDACC MAX-DOAS Central Processing Facility

Date: 02/04/2020

Version: 2.0

1

5. Questionnaire

We kindly ask you to fill in the questionnaire below indicating your interest in participating in the NDACC MAX-DOAS Service and its Central Processing Facility. For those who responded to the FRM$_4$DOAS questionnaire released in May 2017, we also ask you to fill in the questionnaire with updated information about your MAX-DOAS instrument(s).

Personal details:

PI name :.....

Position :.....

Institute + address :.....

:.....

:.....

:.....

:.....

E-mail :.....

Q1/ Are you interested in providing radiance spectra (level-1 data) from your MAX-DOAS instrument(s) to the NDACC MAX-DOAS Central Processing Facility taking advantage of common community algorithms? If yes, go to Q2; if not, please explain the reason(s) why you are not interested:

y/n

.....

Q2/ What are the locations (site name + coordinates) of the MAX-DOAS instruments from your institute that could provide level-1 data to the NDACC MAX-DOAS Central Processing Facility? For each site/instrument, please indicate whether it is already part of NDACC, provide a general classification of the instrument type (e.g. "research grade system" , "mini-DOAS", "EnviMes", "Airyx", "Pandora", etc + pointing/imaging CCD/PDA; outdoor/indoor instrument; manufacturer/custom-built; see example below), and provide instrument specifications according to the Table below:

Site 1: site_name, country (lat, long); NDACC-affiliated site ? ; instrument type

Site 2: site_name, country (lat, long); NDACC-affiliated site ? ; instrument type

Site 3: site_name, country (lat, long); NDACC-affiliated site ? ; instrument type

Site 4: site_name, country (lat, long); NDACC-affiliated site ? ; instrument type

.....

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Example:

Site 1: Bremen, Germany (53°N, 9°E), NDACC-Yes, research grade, pointing, CCD, indoor, custom-built

Instrument specifications (mark relevant specification with a cross):

	Site 1	Site 2	Site 3	Site 4
UV spectral range (300-400nm)*	*x (310-390)*			
Visible spectral range (400-550nm)*				
Depolarizing fiber(s)				
Fiber light mixing				
Detector(s) cooling				
Instrument thermal stabilization				
Elevation scan capability				
Azimuthal scan capability				
Direct-sun pointing capability				

*Please also mention the spectral range in nm (see example in *italic*).

Comments (optional):

.....

Q3/ Which of the following parameters or procedures are part of your instrument characterization/calibration?

(mark relevant specifications with a cross):

	Site 1	Site 2	Site 3	Site 4
Slit function (ISRF)				
Wavelength registration				
Dark signal				
Spectral stray-light				
Detector non-linearity				
Detector interpixel variability				
Field of view				
Elevation angle				
Radiometric calibration				

Comments (optional):

.....

Q4/ How do you operate your instrument(s)?

Instrument operation (mark relevant specification(s) with a cross):

	Site 1	Site 2	Site 3	Site 4
Automatic operation				

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WP1530: CPS Verification and Validation

Tasks:

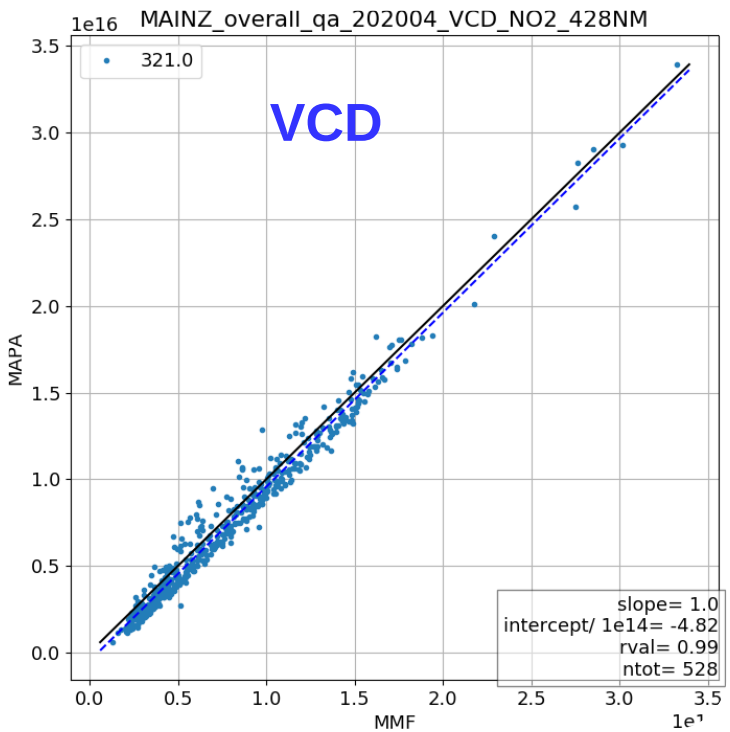
- To verify the tropospheric and stratospheric products from CPS

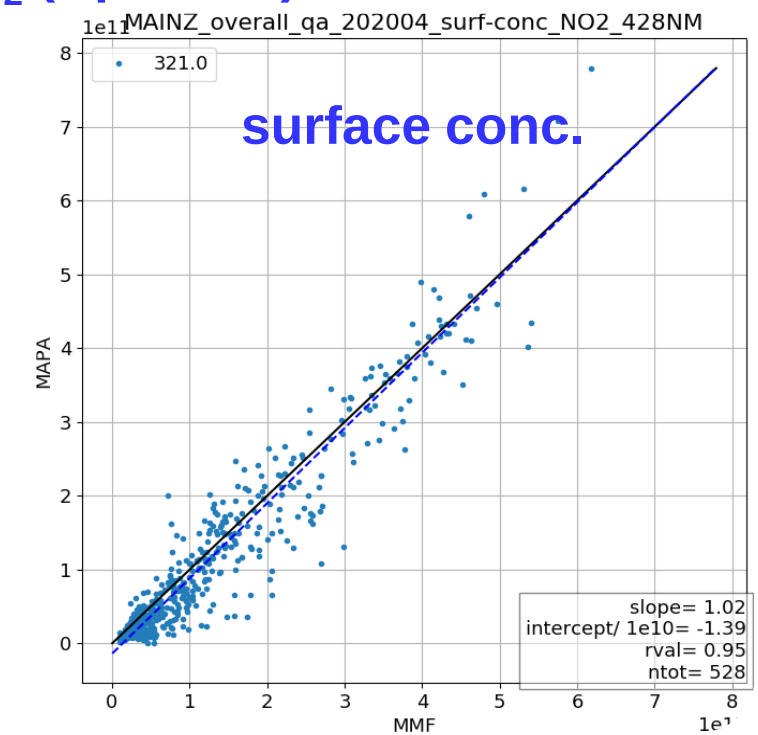
WP1530: CPS Verification and Validation

Tasks:

- To verify the tropospheric and stratospheric products from CPS

Mainz NO_2 (Apr 2020)





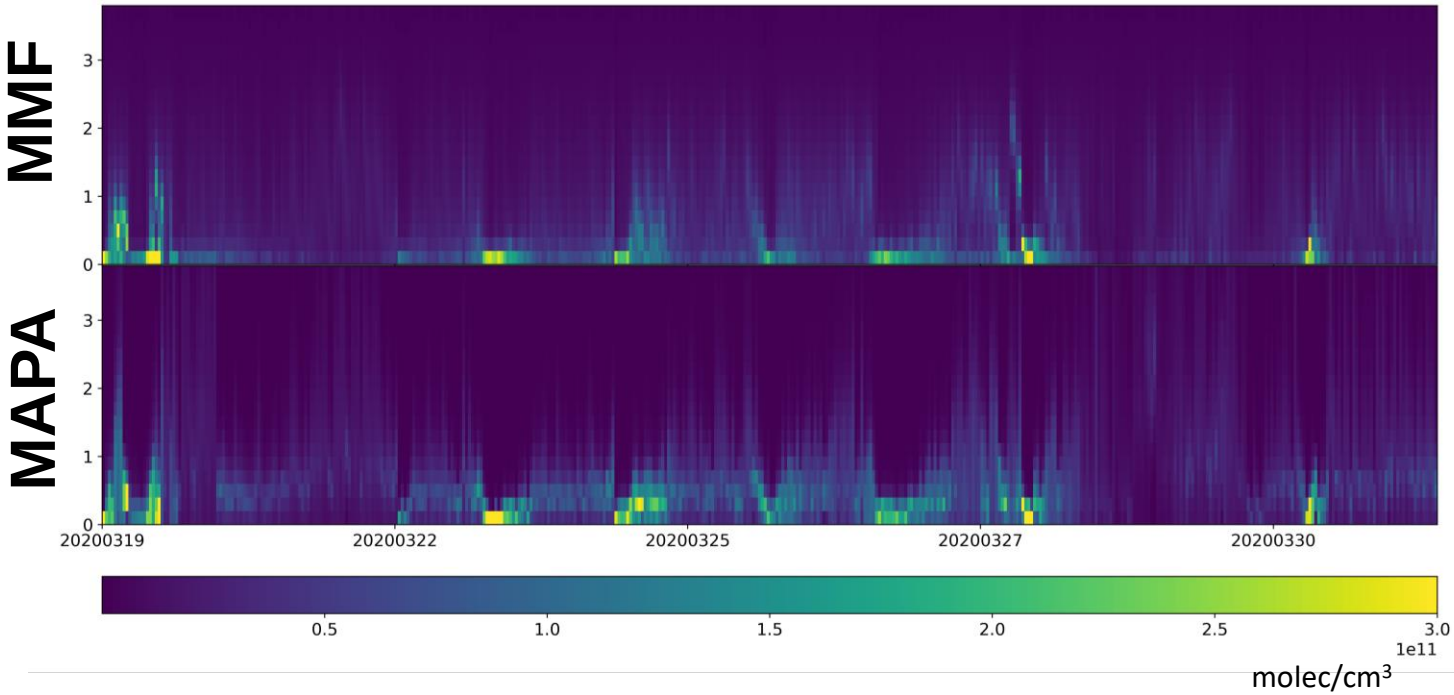
Friedrich and Richter talks ~10h35

WP1530: CPS Verification and Validation

Tasks:

- To verify the tropospheric and stratospheric products from CPS

Mainz NO_2 (Mar 2020)



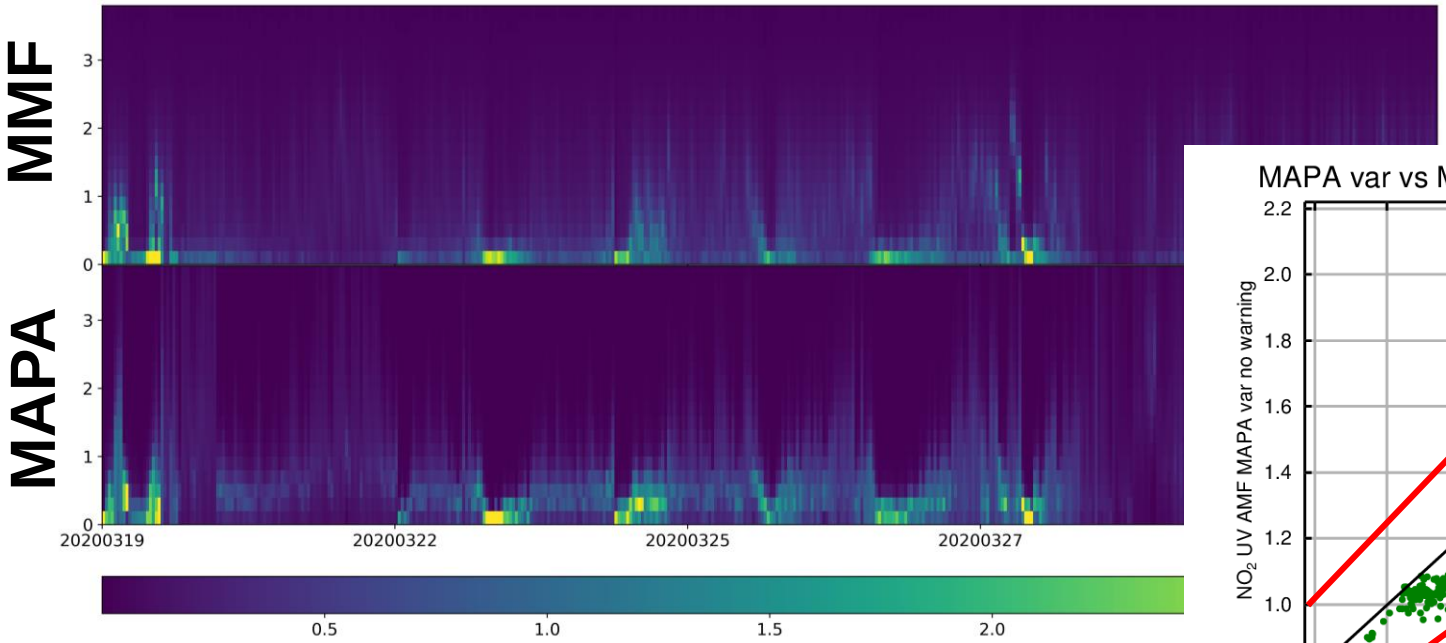
Friedrich and Richter talks ~10h35

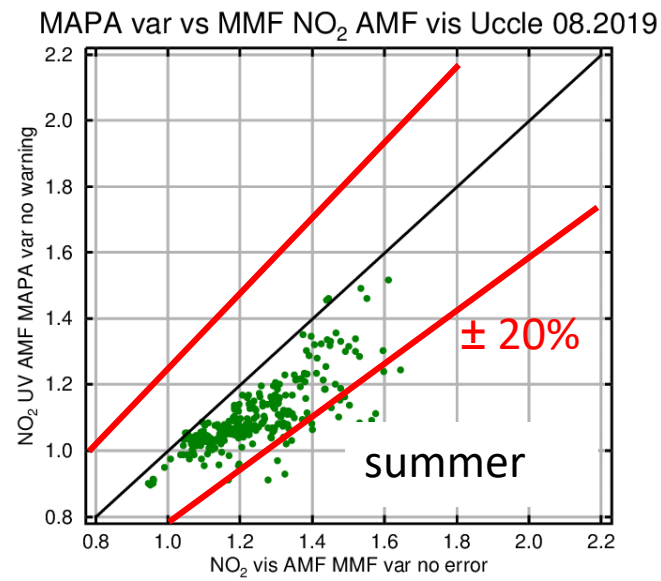
WP1530: CPS Verification and Validation

Tasks:

- To verify the tropospheric and stratospheric products from CPS

Mainz NO_2 (Mar 2020)





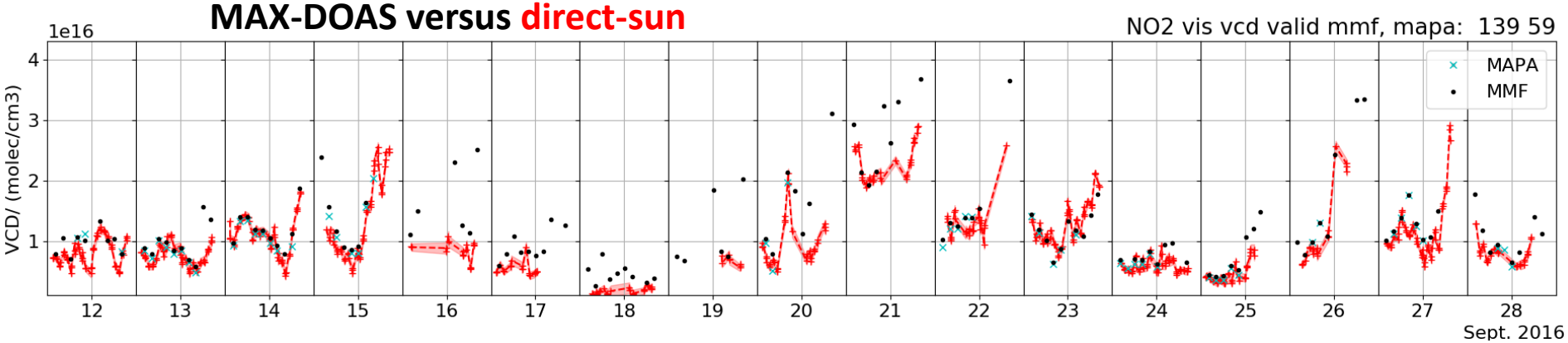
WP1530: CPS Verification and Validation

Tasks:

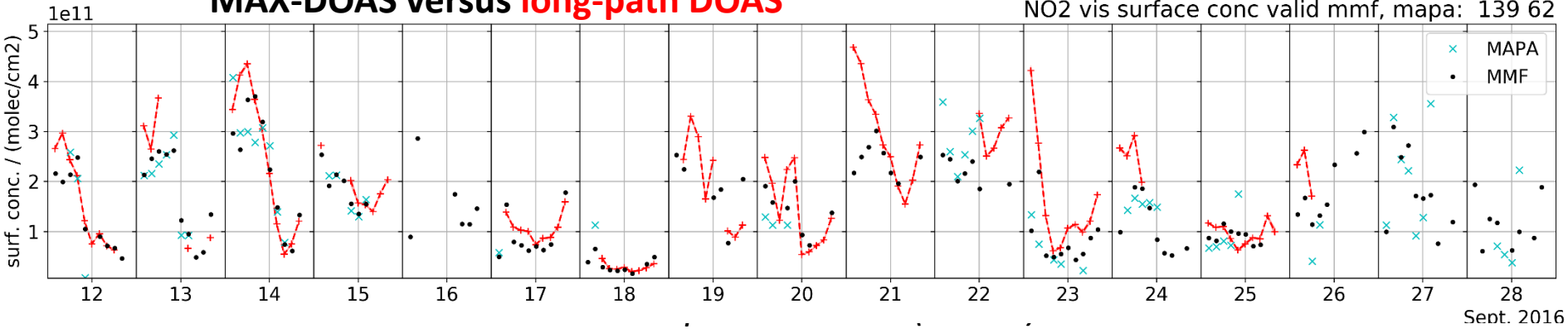
- To verify the tropospheric and stratospheric products from CPS

CINDI-2 NO_2

MAX-DOAS versus direct-sun



MAX-DOAS versus long-path DOAS

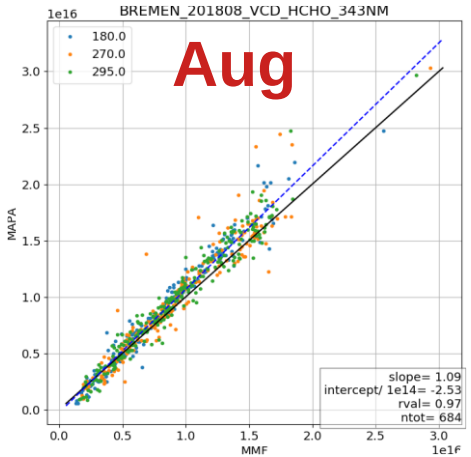


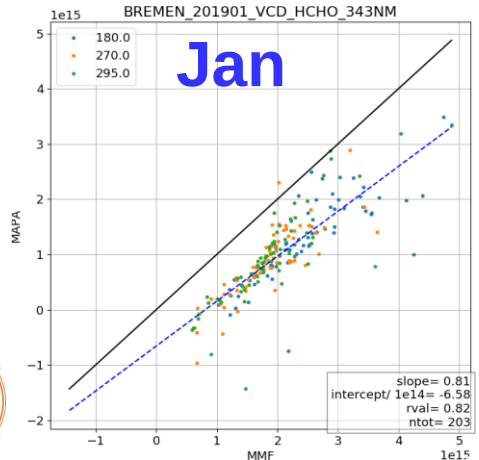
WP1530: CPS Verification and Validation

Tasks:

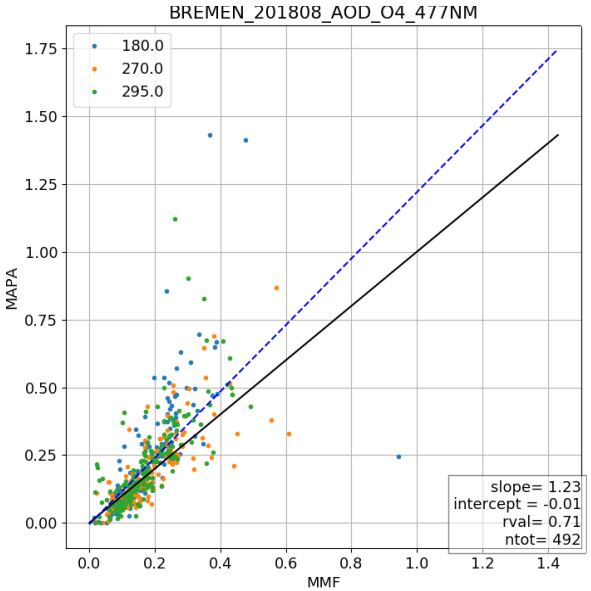
- To verify the tropospheric and stratospheric products from CPS

Bremen HCHO VCD





Bremen AOD



Friedrich and Richter talks ~10h35

WP1530: CPS Verification and Validation

Tasks:

- To verify the tropospheric and stratospheric products from CPS

❑ NO_2 product is in good shape.

❑ HCHO and AOD: discrepancies between MAPA and MMF

➢ *Products not mature enough to be released at this stage.*

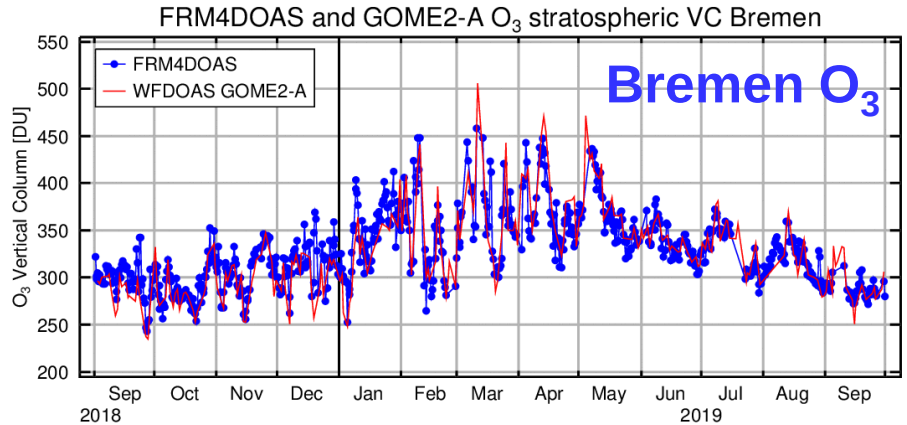
➢ *More investigations are needed.*

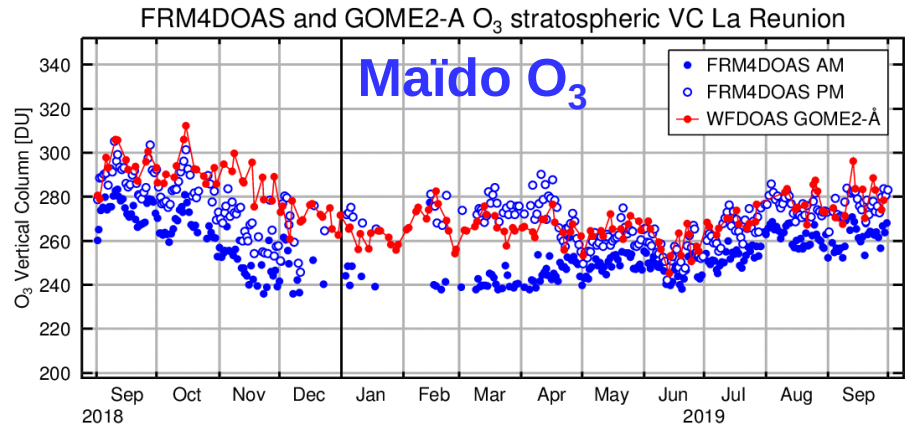
Friedrich and Richter talks ~10h35

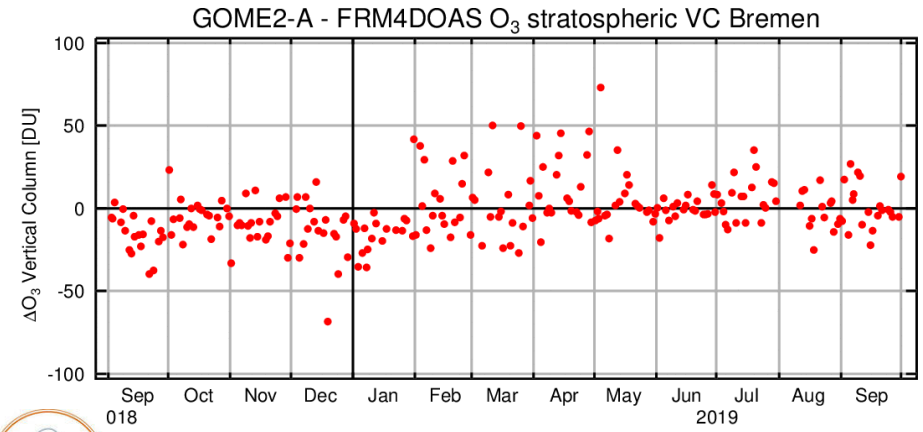
WP1530: CPS Verification and Validation

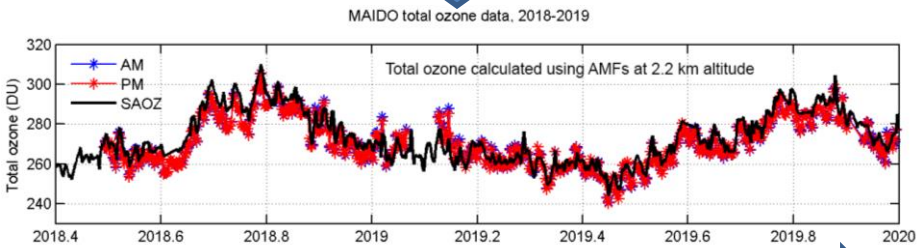
Tasks:

- To verify the tropospheric and stratospheric products from CPS







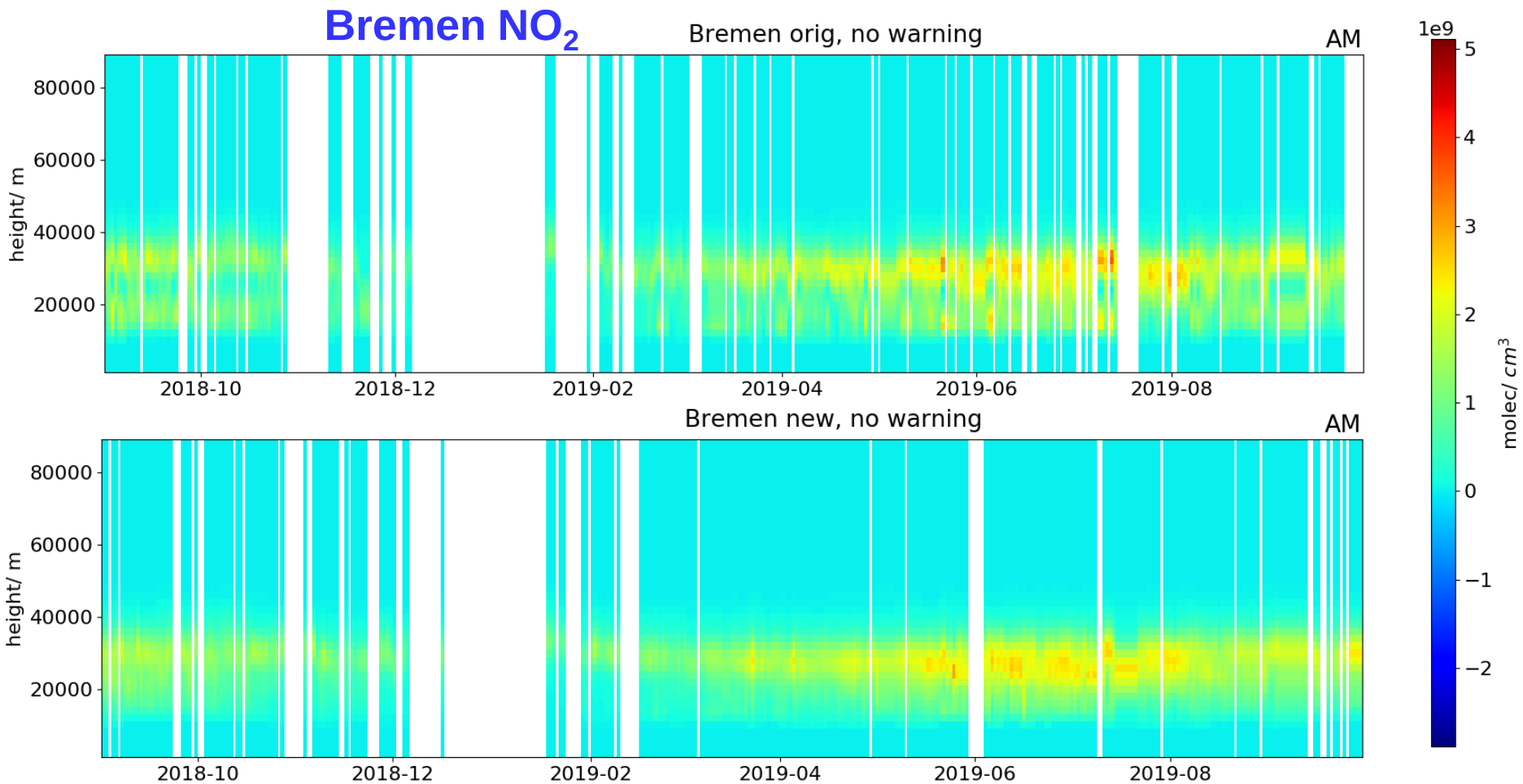


Richter and Hendrick talks ~11h05

WP1530: CPS Verification and Validation

Tasks:

- To verify the tropospheric and stratospheric products from CPS



WP1530: CPS Verification and Validation

Tasks:

- To verify the tropospheric and stratospheric products from CPS

- ❑ Total O_3 column retrieval is in good shape.
  - ➢ *Require twilight measurements in 450-550 nm spectral range (at least 450-520 nm)*

- ❑ Stratospheric NO_2 vertical profile retrieval not yet mature.
  - ➢ *Better estimation of the random uncertainty on NO_2 DSCDs*
  - ➢ *Further investigations on OEM retrieval settings*

Richter and Hendrick talks ~11h05

WP1530: CPS Verification and Validation

Tasks:

- To verify the tropospheric and stratospheric products generated by the operational CPS

- To create a test suite of level-1 files with different main and ancillary contents (T, p, aerosol properties) and check the corresponding response of the CPS

U. Friess talk ~11h25

WP1530: CPS Verification and Validation

Tasks:

- To verify the tropospheric and stratospheric products generated by the operational CPS
- To create a test suite of level-1 files with different main and ancillary contents (T, p, aerosol properties) and check the corresponding response of the CPS
- To estimate the performance of the CPS (computing time, storage capacity)

M. Friedrich talk ~9h40

Concluding remarks

- **All main development steps towards the demonstration of the NDACC MAX-DOAS Service achieved:**
  - ✓ *Optimisation of the Phase I prototype processor and its conversion into an automated central processing facility*
  - ✓ *Assessment of products maturity (TROPONO2 and TOTALO3 ok) and central processor performance*
  - ✓ *Set-up of NDACC and EVDC databases and file submission testing*
  - ✓ *Creation of the "administrative" framework for service upscaling*
  - ✓ *Assessment of NDACC MAX-DOAS Service readiness (stations/products)*

MAX-DOAS Service Readiness (status on 18/05/2020)

instr_num	station_name	affiliation	geometry	Level-1 daily sub	STRATO NO2	TOTAL O3	TROPO NO2	TROPO HCHO
1669	XIANGHE	BIRA.IASB	maxdoas	x		x	x	
1670	UCCLE	BIRA.IASB	maxdoas	x	Instrument currently dismantled			
1671	HARESTUA	BIRA.IASB	zenith	x		x	NA	
1672	NY.ALESUND	IUP	maxdoas	x		x	x	
1673	BREMEN	IUP	maxdoas	x		x	x	
1674	ATHENS	IUP	maxdoas	x		x	x	
1675/ 1684	DEBILT	KNMI	maxdoas	m		NA	x	
1676	MAINZ	MPIC	maxdoas	x		NA	x	
1677	LAUDER	NIWA	maxdoas	t	data flow not yet established			
1678	NEUMAYER	UHEIDELBERG	maxdoas		data flow not yet established			
1679	HEIDELBERG	UHEIDELBERG	maxdoas	x		x	x	
1681	LA.REUNION.MAIDO	BIRA.IASB	maxdoas	x		x	MTS	
1683	THESSALONIKI	AUTH	maxdoas	m		x	x	
1698	IZANA	INTA	maxdoas	w		x	MTS	

t: only level-1 test file submitted so far
w: ~weekly submission of level-1 files
m: ~monthly submission of level-1 files

x: retrieval results still to be verified
NA: algorithm not applicable
MTS: mountain-top site

FRM4DOAS

Concluding remarks

- **All main development steps towards the demonstration of the NDACC MAX-DOAS Service achieved:**
  - ✓ *Optimisation of the Phase I prototype processor and its conversion into an automated central processing facility*
  - ✓ *Assessment of products maturity (TROPONO2 and TOTALO3 ok) and central processor performance*
  - ✓ *Set-up of NDACC and EVDC databases and file submission testing*
  - ✓ *Creation of the "administrative" framework for service upscaling*
  - ✓ *Assessment of NDACC MAX-DOAS Service readiness (stations/products)*
- **Launch of the service in demonstration mode (only for testing/no operational commitments) before the Copernicus project KO**
- **Future MAX-DOAS R&D and operational activities as part of the new ESA and Copernicus projects to be discussed (-> tomorrow session)**

Thank you for your attention !