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

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MAX-DOAS Aerosol Algorithm TIP

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Authors

Martina M. Friedrich[1]
Steffen Beirle[3]
Thomas Wagner[3]
Udo Frieß[2]
Caroline Fayt[1]
Michel Van Roozendael[1]

[1] Belgian Institute for Space Aeronomy (BIRA-IASB)
[2] Institut für Umweltphysik, Universität Heidelberg (IUPHD)
[3] Max Planck Institute for Chemistry (MPIC)

Document change record

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0.1	June 4, 2025	all	Initial version

Contents

Acronyms and abbreviations

AOD Aerosol Optical Depth.

BIRA-IASB Belgian Institute for Space Aeronomy.

CAMS Copernicus Atmosphere Monitoring Service.

CPS Central processing system.

DSCD Differential Slant Column Density.

FRM4DOAS Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations.

GEOMS Generic Earth Observation Metadata Standard.

IUPHD Institut für Umweltphysik, Universität Heidelberg.

LUT Look-up table.

MAPA MAinz Profile Algorithm.

MMF Mexican MAX-DOAS Fit.

MPIC Max Planck Institute for Chemistry.

PM person month.

SF O_4 scaling factor.

TIP Technical implementation plan.

WL work load.

WP Work package.

1 Introduction

This Technical implementation plan (TIP) describes the implementation changes to account for the changes proposed in **[RD-1]** to the algorithms that are implemented in the Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations (FRM4DOAS) Central processing system (CPS) for the retrieval of tropospheric vertical aerosol extinction profiles and Aerosol Optical Depth (AOD). It is part of Work package (WP)-3 of FRM4DOAS-2.0.

The nature of these changes has been described in **[RD-1]**. This document describes the needed steps for implementation in the CPS.

The goal in this WP of the follow-up project FRM4DOAS-2.0 was to include aerosol tropospheric AOD together with the vertical aerosol extinction profile as a stand-alone product, as described in **[AD-1]**. The final product is the creation of an aerosol Generic Earth Observation Metadata Standard (GEOMS) file.

2 Requirements, modifications and extensions for the implementation of the new aerosol product in the CPS

The work needed for implementing the changes presented in **[RD-1]** is detailed in this section. Estimates for the work load (WL) of the different tasks outlined in the subsections of this section are summarized in Table 1.

Table 1: Identified tasks needed for implementing the aerosol product in the CPS and estimates of the WL, given in PM

Task	Affected modules	WL/PM	Institute
Ensuring consistence between MAPA AOD and extinction profile + testing	`FRM4DOAS_output_aerosol_vX.yml`	0.5	MPIC/ BIRA-IASB
Implementing the new flagging scheme in MMF + testing	`MMFprofiling.py`, `mmf_settings.yml`	1	BIRA-IASB
Implementing the use of SFs from MAPA in MMF and updating *a priori* settings + testing	`ProfilePreprocessBira.py`, `MMFprofiling.py`, `MAPA.py`, `MMF.py`, `GENERAL config.yaml`, `setup.txt`	1.5	BIRA-IASB
Implementing the creation of the aerosol GEOMS output + testing	`GeomsOut.py` and configuration file creation	1	BIRA-IASB

2.1 Changes to MAPA configuration file

The changes to MAPA only require a change in the `FRM4DOAS_output_aerosol_vX.yml` file. Specifically, the change of the MAPA key for `aerosol_optical_depth` from `c_best` to `c_weighted_mean`. This ensures that the variable `aerosol_optical_depth` matches the

variable `aerosol_extinction_profile` (i.e. the AOD can be larger, due to the contribution above 4 km, but it cannot be smaller than the integrated profile).

Likewise, sets of variables using `c_best` and `profile_best` are included as `aerosol_extinction_profile_best_matching_parameter_representation` and `aerosol_optical_depth_best_matching_parameter_representation`.

For completeness, also the other Look-up table (LUT) best-match parameters (for h, s and SF, see Beirle et al. (2019)) are included. Additionally, the set of reported flags is extended to include all MAPA flag components.

It needs to be ensured that the correct values (weighted mean) are taken for the comparison with MMF to create an overall flag, similar to the one already in place for NO_2.

2.2 Changes to MMF configuration files and code

2.2.1 configuration files

Changes for flagging

For MMF the changes involve two configuration files. For the changes on the flagging, the file in question is *mmf_settings.yml*, and here specifically the section `flag_limits` and `settings`. The new parameters for

- rms warning and error limits
- a priori variation factor for stability test
- stability warning and error limits
- aod warning and error limits

can simply be adjusted. The additional limits to include the new error flag components as described in **[RD-1]**, need to be included in the same file:

- SF limits for error
- error limits on the third derivative of profile
- error limits for the profile fraction above 3 km

These new flag components and the functionality of boosting the scaling of the S_a matrix by the inverse of the *a priori* variation factor, requires a code change and is further described in Sect.2.2.2.

Changes for *a priori* settings in MMF

The changes involving changes of the *a priori* are partly in the instrument specific settings[1] and hence need to be changed in each of them: The scale factor α and the correlation length γ (c.f. **[RD-1]**) can be changed directly in the `setup.txt` files in each station. The new *a priori* extinction profile shape file with the adapted scale height h_s has to be created once off-line with an arbitrary integrated AOD amount (the profile is scaled internally to the one provided in the default or station specific settings).

[1] except for the default AOD which can be set directly in the `frm4doas_tropo.cnf` file, or per-instrument in `station_tropo_config_version.yaml` file

2.2.2 Code changes

Changes for flagging

In order to include the up-scaling of α (for the S_a matrix) in the stability tests, an according step needs to be implemented in the component `MMFprofiling.py` that manipulates on the fly the aforementioned `setup.txt` files read in by the fortran core of MMF. This will include extending the list of input parameters in the instance method `writesetup` of the MMF object, as well as the adjustment of α in the *run_mmf* instance method of MMF in the `LOW_APRI` section.

To include the new flag components, the function *new_make_flag* in `MMFprofiling.py` needs to be extended to check for the components listed above in Sect.2.2.1. Apart from the logic to include, this requires to pass the SF from MAPA. This introduces an a-symmetry of how the two retrieval codes are handled and is of the level of the pre-processing. It is hence described in Sect.2.3.

Changes for applying MAPA SFs in MMF

Passing the SF directly from the pre-processing routine enables that the measured Differential Slant Column Densities (DSCDs) for O_4 can be adjusted within MMF and do not need to be changed in the pre-processing part. It needs to be decided whether the simulated DSCDs are up-scaled (down-scaled in the case of SF>1) similarly as internally done in MAPA, or whether a second set of measured DSCDs applying the SF should be provided within the MMF group.

Applying these SFs inside `MMFprofiling.py` needs to be implemented as a new instance method on the `MMF_MASTER` object, e.g. `adjust_measured_O4_dscds` that multiplies the set of measured O_4 DSCDs with the passed set of SFs.

2.3 Changes to the Pre-processing module and associated configuration files

Changes for applying MAPA SFs in MMF

The current implementation of the pre-processing in `ProfilePreprocessBira.py` treats all tropospheric retrieval codes in the same way and requires a code-specific module, e.g. `MAPA.py` or `MMF.py` to be present to make code-specific adjustments of the input parameters. These modules contain each two functions, one `configure_frm4doas` and one `run_frm4doas`.

The most straight forward way to include the changes is hence to create fully masked SF arrays of the same length as number of scans and include them in the dictionary `Ip` passed to the generic `algo_module.run_frm4doas(Ip)` routine.

Additionally, the SF array needs to be passed back explicitly from the generic function, so that it is updated for consecutive codes that are included. This includes hence changes in each of the `algo_module.run_frm4doas(Ip)` functions. For the `MAPA.run_frm4doas` function this means to extract the SF from the MAPA output dict and use this to update the SF passed initially. For `MMF.run_frm4doas` this means to include the SF information and pass on to the main MMF routine.

In order for MMF to use the filled version of those, the correct order of codes need to be set in the configuration file `GENERAL_config.yaml` in the `SETTINGS/do_algos` section.

Note that codes that run after MAPA are not required to do anything with the supplied SFs, they can be simply ignored in the specific `run_frm4doas` routine.

2.4 GEOMS file creation

2.4.1 New configuration files

A corresponding configuration file mapping the master output file variables to GEOMS variables, similar to that for trace gases, `l2_to_geoms.yaml`, has to be created. It needs to be ensured that all the variables that are listed as mandatory in the template file GEOMS-TE-UVVIS-DOAS-OFFAXIS-AEROSOL-007.csv[2] are extracted correctly. Specifically, as a variable that has no counter-part in the trace gas file, the wavelength needs to be added.

2.4.2 Code changes

A number of routines are involved in the GEOMS file creation for the tropospheric trace gas products, namely:

- `extract_data_tropo`
- `translate_data_tropo`
- `adjust_template_gas_algo`
- `make_geoms_tropo`

It is expected that the `extract_data_tropo` should work directly with the new configuration file for the aerosol product (see Sect.2.4.1), it is however a matter of testing whether this is the case.

Since the output translation is more direct (as opposed to the trace gas conversion that involved for all variables a conversion from number densities to concentration), the translation part is merely a re-ordering.

No name changes in the variables are needed as opposed to the trace gas GEOMS files, hence `adjust_template_gas_algo` should not be needed for the aerosol product.

`make_geoms_tropo` is the wrapper around the other routines. Only slight changes, e.g. a conditional to run `translate_data_tropo`, should need to be implemented.

2.5 Additional work

Test routines testing that the GEOMS output file corresponds to the output reported in the master output file, need to be created, or a sufficiently large number of files have to be compared manually.

Limits for uncertainty ranges have to be defined and communicated to Copernicus Atmosphere Monitoring Service (CAMS)27 responsible for quality monitoring.

[2] https://git.nilu.no/geoms/templates/-/blob/master/GEOMS-TE-UVVIS-DOAS-OFFAXIS-AEROSOL-007.csv

3 Optional additional adjustment of retrieval grid

In **[RD-2]**, as a task with low priority it was recommended to change the retrieval grid to one that has a higher resolution close to the surface. This has not been tested in **[RD-3]**. Should this eventually be implemented, then this requires changes in various configuration files:

- `frm4doas_tropo.cnf` this sets the grid on which the output is delivered
- `setup.txt` In MMF the internal grid is currently set to the same resolution as the output grid, however, the retrieval grid can be changed independently. If the output grid is to be changed to a finer resolution close to the surface, it is recommended to include also a finer resolution close to the surface for MMF internal grid. While MMF can handle irregular grids, huge differences between layer thicknesses have to be avoided since those introduce artifacts.
- MAPA should directly be able to produce the output on any supplied input grid. However, currently the supplied height grid is ignored. In order to change the output grid, a slight update of MAPA is therefore needed. Since MAPA is undergoing a major update, it is recommendable however to directly switch to the new MAPA version. The implementation of this in the CPS however constitute a major work since additional python libraries need to be installed and the interfaces (c.f. the above mentioned `MAPA.py` module) need to be adjusted.

4 References

[RD-1] FRM4DOAS-2.0. *ATBD*. Deliverable D3.4. FRM4DOAS-2.0.

[RD-2] FRM4DOAS-2.0. *Technical Note*. Deliverable D3.2. Deliverable D3.2. FRM4DOAS-2.0.

[RD-3] FRM4DOAS-2.0. *Validation Report*. Deliverable D3.3. FRM4DOAS-2.0.

[AD-1] ESA/ESRIN. *Statement of Work*. ESA Express Procurement - [EXPRO] ESA-EOPG-EOPGMQ-SOW-23. FRM4DOAS-2.0, Mar. 2021.

Beirle et al. (2019) S. Beirle, S. Dörner, S. Donner, J. Remmers, Y. Wang, and T. Wagner. "The Mainz profile algorithm (MAPA)". In: *Atmospheric Measurement Techniques* 12.3 (2019), pp. 1785–1806. DOI: 10.5194/amt-12-1785-2019.