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

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Deliverable D1.5:

Technical implementation plan (TIP)

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Content

Acronyms and abbreviations

Acronyms and abbreviated terms that are specific for this document can be found below.

CPS	Central Processing System
CTM	Chemistry transport Model
DISORT	Discrete-Ordinate Radiative Transfer model
DOAS	Differential Optical Absorption Spectroscopy
DSCD	Differential Slant Column Density
EDE	Extra-DSCD error
FRM_4DOAS	Fiducial Reference Measurements for Ground-Based DOAS Air-Quality Observations
JPL	Jet Propulsion Laboratory
LUT	Look-up Table
RTM	Radiative transfer model
SLIMCAT	Single Layer Isentropic Model of Chemistry And Transport
SZA	Solar zenith angle
UT	Universal Time
WF	Weighting functions

1 Introduction

This document presents the essential technical steps needed for the implementation of the stratospheric NO_2 product consolidation approaches in the CPS. Those approaches, developed as part of WP1 and extensively described in Deliverable D-1.5, include:

- The extra-DSCD error approach
- The use of ±15-day averaged weighting functions, twilight NO_2 profile variation, and a priori profile
- The calculation and use of optimised NO_2 profile diurnal variation simulation results
- The implementation of a correction for the Earth's sphericity on the NO_2 weighting functions (WF)
- The revised uncertainty budget

Estimations of the workload and computational cost corresponding to this consolidation effort are also provided.

2 Extra-DSCD error approach

Involved CPS routine and configuration files:

- *retrieval_no2_profile_strato_v_02_0.py*: main Python routine for stratospheric NO_2 profile retrieval
- *frm4doas_strato.cnf* and *strato_input_config.yml* configuration files

Main implementation steps:

In the *retrieval_no2_profile_strato* function of the *retrieval_no2_profile_strato_v_02_0.py* routine:

- Perform a first profile retrieval with the standard DOAS fit errors.
- For each measurement SZA in the 75-93°SZA interval, calculate the difference between the measured DSCD and the simulated DSCD using this profile. This difference is called extra-DSCD error (EDE).
- For each measurement SZA in the 75-93°SZA interval, check if the EDE is larger by more than a threshold factor than the standard DOAS fit error. This threshold factor (chosen value: 10) has to be defined in the *frm4doas_strato.cnf* configuration file.
- For each measurement SZA for which the above check condition is fulfilled, replace the standard DOAS fit error by the EDE for the construction of the measurement noise S_ϵ matrix.
- Create a specific variable EDE for reporting the EDE. The fill value '0' is used for SZAs at which the standard DOAS fit error is modified. This variable has to be defined in the *strato_input_config.yml* configuration file and is reported in the level-2 netCDF output file.
- If the standard DOAS fit error is modified for at least one measurement SZA, the *retrieval_no2_profile_strato* function is called for a second retrieval step using the new DSCD errors.

3 Use of ±15-day averaged weighting functions, NO_2 profile twilight variation, and a priori profile

Involved CPS routine:

- *retrieval_no2_profile_strato_v_02_0.py*: main Python routine for stratospheric NO_2 profile retrieval

Main implementation steps:

In the *retrieval_no2_profile_strato_v_02_0.py* routine:

- Modify the *find_day_idx* function in order to select the indices (idx) of the weighting function LUT day grid which correspond to the measurement local day ±15 days time interval. A variable holding all corresponding indices is created, idxday_vec.
- Create a loop (over each idx in idxday_vec) in the constructor *__init__* of each measurement object and extract the NO_2 profile diurnal variation and WF. Then still in this loop, interpolate both at the measurement SZAs and interpolate the NO_2 profile diurnal variation at 90°SZA in order to get the a priori profile.
- In the constructor *__init__* of each measurement object, calculate averages of interpolated weighting functions, twilight NO_2 profile variations, and a priori profiles. Then, scale the averaged weighting functions with the averaged NO_2 profile twilight variation normalised with respect to 90°SZA.

4 Calculation and use of optimised NO_2 weighting function and profile diurnal variation LUTs

Main implementation steps:

- Calculation of new NO_2 vertical profile diurnal variations using the PSCBOX stacked box photochemical model:
  - Initialised daily at 20 independent altitude levels (between ~10 and ~55 km of altitude) with 0h UT meteorological and chemical fields from the 3D CTM SLIMCAT (run n°509 for year 2009) for the following latitudes (longitude is set to 0°): 75°N, 70°N, 65°N, 60°, 55°N, 50°N, 45°N, 35°N, 25°N, 15°N, 5°N, 5°S, 15°S, 25°S, 35°S, 45°S, 50°S, 55°S, 60°S, 65°S, 70°S, 75°S
  - Reactions rate constants from JPL Evaluation n° 19-5 (Burkholder et al., 2020; https://jpldataeval.jpl.nasa.gov/pdf/NASA-JPL%20Evaluation%2019-5.pdf)
  - NO_2 photolysis rate multiplied by a factor of 0.9 (see Deliverable D-1.1).
- Calculation of new NO_2 weighting function LUTs with the UVSPEC/DISORT RTM initialised with the new NO_2 vertical profile diurnal variations. The entry parameters are the same as for the LUTs currently implemented in the CPS, i.e.:
  - Latitude: 75°N, 70°N, 65°N, 60°, 55°N, 50°N, 45°N, 35°N, 25°N, 15°N, 5°N, 5°S, 15°S, 25°S, 35°S, 45°S, 50°S, 55°S, 60°S, 65°S, 70°S, 75°S
  - Day number: 1 to 361 with a 5-day step and 365
  - Wavelength: 360, 425, and 460 nm

Those LUTs also contain the corresponding NO_2 profile diurnal variations used for the calculation of the weighting functions. These diurnal variations are used in the retrieval algorithm for normalizing the weighting functions with respect to the retrieval SZA (90°; see Deliverable D-1.1).

- Conversion of the native LUTs which are in an ascii format into a single nc file.
- Loading of the new LUT nc file by the profiling algorithm routine, i.e. *retrieval_no2_profile_strato_v_02_0.py* and appropriate WF and NO_2 diurnal variation extractions.

5 Implementation of a correction for the Earth's sphericity on the NO_2 WF

Involved CPS routine:

- *retrieval_no2_profile_strato_v_02_0.py*: main Python routine for stratospheric NO_2 profile retrieval

Main implementation steps:

- Create a netCDF file containing the correction factors for Earth's sphericity derived from the intercomparison exercise of full spherical and pseudo-spherical RTMs (see Deliverable D-1.1). Those correction factors are provided at two wavelengths (326 and 460nm) and for the following set of SZAs: 0 to 65° with 5° step, then 66 to 95° with 1° step.
- In the *retrieval_no2_profile_strato_v_02_0.py* routine:
  - Create a function for (1) loading the correction factors nc file and (2) interpolate the correction factors at the measurement wavelength and SZAs.
  - Pass the interpolated correction factors to the *interpolate_wf* function and correct the WFs accordingly.

6 Implementation of revised uncertainty budget

Involved CPS routines and configuration files:

- *retrieval_no2_profile_strato_v_02_0.py*: main Python routine for stratospheric NO_2 profile retrieval
- *strato_input_config.yml* configuration file

Main implementation steps for the forward model parameter errors:

- In the AM_PM group of the *strato_input_config.yml* configuration file, initialize forward model parameter error variables for both profile and VCD (*prof_fmodel_err* and *no2_col_err_f* variables, respectively).
- Create a netCDF file containing the relative forward model parameter errors. Those errors correspond to the addition in Gaussian quadrature of the forward model parameter errors coming from Preston et al. (1997) and from the sensitivity tests on NO_2 photolysis rate (jNO_2 x 0.9) and Earth's sphericity (see Deliverable D-1.1)
- In the *retrieval_no2_profile_strato_v_02_0.py* routine:
  - Create a function for loading the relative forward model parameter errors nc file.

– Pass the relative forward model parameter errors data as argument of the *do_retrieval* function and calculate the forward model parameter errors on profile and VCD in this function.

Main implementation steps for the EDE in the uncertainty budget:

- Done in a transparent way since automatically included in the measurement noise S_ε matrix (see Sect. 2).

7 Overall testing step

An overall testing of the consolidated version of the profiling algorithm will be performed. It will consist in checking the output level-2 nc files for a selection of stations and assessing any impact on the performance (computing time, storage) of the CPS.

8 Workload and computational costs

Table 1 summarises the workload and computational costs related to the implementation of the different consolidation approaches and corresponding testing steps and the overall testing of the new version of the algorithm.

Consolidation approach	Workload (person.day)	Computational cost with respect to the current processing	
		Computing time	Storage
Extra-DSCD error + testing	2	The computing time for sunrise and sunset profile retrievals is 15s. This time will be multiplied by two if a second retrieval step including EDE is needed.	Daily level-2 nc files larger by a few KB than the current ones
±15-day averaged weighting functions, NO_2 profile twilight variation, and a priori profile + testing	2	<5s	No impact
Calculation of new weighting function and NO_2 profile diurnal variation LUTs based on updated photochemical box-model run + LUTs verification + testing	5	1 month for the off-line calculation of the LUTs; no impact on the CPS processing time	280 MB (same size as the current LUTs)
Implementation of Earth's sphericity correction on NO_2 WF + testing	2	<1s	No impact
Implementation of revised uncertainty budget + testing	2	<1s	Daily level-2 nc files larger by a few KB than the current ones
Overall testing step	5	N/A	N/A

Table 1. Estimates of the workload and computational costs corresponding to the different stratospheric NO_2 product consolidation approaches and the overall testing of the new version of the algorithm.

9 References

Preston, K. E., R. L. Jones, and H. K. Roscoe, Retrieval of NO_2 vertical profiles from ground-based UV-visible measurements: Method and validation, J. Geophys. Res., 102 (D15), 19.089-19.097, 1997.