



Derived tropospheric column data

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Acronyms and abbreviations

AVK	averaging kernel
CO	carbon monoxide
CH ₄	methane
FTIR	Fourier transform infrared spectroscopy
GCTM	global chemistry and transport model
GEOMS	generic earth observation standard
hdf	hierarchical data format
IZO	Izaña
JFJ	Jungfraujoch
MAXDOAS	multi axis differential optical absorption spectroscopy
NO ₂	nitrogen dioxide
O ₃	ozone

1. Introduction

This deliverable comprises the tropospheric reference data that were developed within WP5 for the two NORS demonstration sites Jungfraujoch and Izaña. These reference data consist of tropospheric vertical profiles that were obtained by merging in-situ data at the observatories and model data. The details of the merge procedure are outlined in deliverable **D5.1**. Note, that while the reference profiles extend to the top of the column retrieved by remote sensing, they have no reference character above 16 km where they purely consist of model data. The influence of surface in-situ observations is limited to below this altitude.

Available data currently, status 2013-11-01, comprise CO, CH₄ and O₃ profiles at the times of available FTIR observations at the two sites for the years 2009 to 2011. Depending on the trace gas up to three different global chemistry and transport model (GCTM) results were used as initial conditions for the detailed transport simulations, which were carried out with the Lagrangian particle dispersion model FLEXPART in backward mode. Reference profiles were generated for any of these large-scale models.

Currently, a total of 36 yearly data files of reference profiles are available in hdf4 format from Empa's NORS website (<http://lagrange.empa.ch/NORS/data>).

Reference data for MAXDOAS measurements of O₃ and NO₂ are expected to become available as soon as the original MAXDOAS data is finally processed and made available by the project partners.

2. Data description

In the following the term “data file” refers to an individual hdf file, while “dataset” refers to a variable within a data file.

The original data structure of the underlying remote sensing data files was kept and the datasets relevant for the tropospheric profile retrieval were retained. Additional datasets in the original data files that contained either no valid data or data not relevant for the generation of the reference profiles were discarded in order to keep file sizes as small as possible and avoid duplication. Since the original data files follow the GEOMS metadata standard, the generated reference data files follow these standards as closely as possible.

Since the transport simulations required for the generation of the reference dataset had a minimal temporal resolution of 1 hour, remote sensing data were aggregated to hourly intervals before the generation of reference data. Hence, hourly mean values of the relevant remote sensing datasets are stored in the present data files. This concerns the hdf datasets

- ANGLE.SOLAR_ZENITH.ASTRONOMICAL
- ANGLE.SOLAR_AZIMUTH.ASTRONOMICAL
- <SPEC>.MIXING.RATIO_ABSORPTION.SOLAR
- <SPEC>.MIXING.RATIO_ABSORPTION.SOLAR_APRIORI
- <SPEC>.MIXING.RATIO_ABSORPTION.SOLAR_AVK
- PRESSURE_INDEPENDENT
- TEMPERATURE_INDEPENDENT
- SURFACE.PRESSURE_INDEPENDENT
- SURFACE.TEMPERATURE_INDEPENDENT

Where <SPEC> stands for the observed trace species.

The data files contain 6 additional vertical reference profiles that present different model simulations and in-situ adjustments:

- <SPEC>.MIXING.RATIO_SIMULATED_FLEXPART.<GCTM>
FLEXPART simulated vertical distribution of <SPEC> using global background fields from <GCTM>
- <SPEC>.MIXING.RATIO_SIMULATED.ADJUSTED_FLEXPART.<GCTM>
FLEXPART simulated vertical distribution of <SPEC> using global background fields from <GCTM> and adjusted to in-situ surface observations
- <SPEC>.MIXING.RATIO_SIMULATED.FOLDED_FLEXPART.<GCTM>
FLEXPART simulated vertical distribution of <SPEC> using global background fields from <GCTM>. The profile was folded with the averaging kernels of the remote sensing retrieval.
- <SPEC>.MIXING.RATIO_SIMULATED.ADJUSTED.FOLDED_FLEXPART.<GCTM>
FLEXPART simulated vertical distribution of <SPEC> using <GCTM> global background fields and adjusted to in-situ surface observations and folded with the averaging kernels of the remote sensing retrieval

- **<SPEC>.MIXING.RATIO_SIMULATED_<GCTM>**
Vertical distribution of CO taken from <GCTM> global fields and extracted at the remote sensing sampling volume.
- **<SPEC>.MIXING.RATIO_SIMULATED.FOLDED_<GCTM>**
Vertical distribution of <SPEC> taken from <GCTM> global fields and extracted at the remote sensing sampling volume and folded with the averaging kernel.

Here <GCTM> stands for the global chemistry and transport model from which initial conditions were taken.

The most comprehensive reference profile is the one which uses the detailed transport simulations and adjusts these according to the surface in-situ observations: **<SPEC>.MIXING.RATIO_SIMULATED.ADJUSTED_FLEXPART.<GCTM>** and **<SPEC>.MIXING.RATIO_SIMULATED.ADJUSTED.FOLDED_FLEXPART.<GCTM>**. The other profiles are provided for comparison reasons. Reference and folded (by AVK) reference profiles are provided. The first allow the direct comparison with other model data while the latter should be used as a reference for the comparison with the profiles obtained by remote sensing.

Detailed transport simulations with FLEXPART were only carried out for remotely sensed sub-columns below 16 km above sea level. Above this altitude the reference profiles contain the values directly interpolated from the GCTM.

3. Data dissemination

The data files are available on a NORS designated web service at Empa (<http://lagrange.empa.ch/NORS/data>). The access to the data is restricted and requires authorisation. The current user name and password are set to "NORS" and "WP5refdata", respectively. The data files are not stored in subfolders. The file names follow the naming convention:

```
groundbased.NORSreference.<GCTM>_ftir_<SPEC>_empa_<site>_<start date>_<stop date>_<VERSION>.hdf
```

where <site> is one of the demonstration sites Jungfraujoch or Izana, <start date> gives the date and time of the first data entry in the file and <stop date> gives the date and time of the last data entry. <VERSION> gives the version of the data. Currently version 2 (V2) is available.

In addition to the data files, figures characterising the sampled air masses and documenting the in-situ data extraction process can be found in the WP5 results gallery found under http://lagrange.empa.ch/NORS_browser.

4. Expected updates of the data files

Currently 36 reference data files for FTIR observations are available. These comprise the years 2009 to 2011. If during the final comparison with the FTIR data, the need should be felt to extend the comparison period, reference data may be provided for an additional year (2012). If inconsistencies in the in-situ data extraction method should become apparent and require reprocessing, a new version of the reference data may be produced.

Reference data for MAXDOAS observations are currently (2013-11-01) generated and will be added to the download location in due time.