Delta D (δD)

Each file contains data for one day of observation.
File names include date of observation. Their structure is:
SENSOR_PLATFORM_LEVEL_"deltaD"_TYPE_YYYYMMDD_INSTITUTION_VERSION".nc"
where:
SENSOR = IASI, PLATFORM = METOPA or METOPB, LEVEL = L2, TYPE = COLUMN, YYYY = year, MM = month, DD = day, INSTITUTION = ULB-LATMOS, VERSION = VX.Z where X is the version number of the retrieval code and Z the version number of the NetCDF file production

The format of the files is NetCDF4.

The structure of the file header (eg for 2 January 2009) is as follows:

```
netcdf IASI_METOPA_L2_deltaD_20090102_ULB-LATMOS_V201701.0 {
dimensions:
        time = 19344 ;
        nlevels = 13 ;
        navkrows = 26 ;
        navkcols = 26 ;
        nchannels = 233 ;
        nchartime = 16 ;
variables:
        double time(time) ;
                time:long_name = "observation time in seconds since 2007-01-01 00:00:00 UTC" ;
                time:units = "second" ;
                time:standard_name = "time" ;
        char time_string(time, nchartime) ;
                time_string:long_name = "UTC observation time as YYYYMMDDThhmmssZ" ;
        double time_in_day(time) ;
                time_in_day:long_name = "observation time in seconds in the day" ;
                time_in_day:units = "second" ;
        float latitude(time) ;
                latitude:long_name = "latitude" ;
                latitude:units = "degrees_north" ;
                latitude:valid_range = -30., 30. ;
                latitude:standard_name = "latitude" ;
        float longitude(time) ;
                longitude:long_name = "longitude" ;
                longitude:units = "degrees_east" ;
                longitude:valid_range = -180., 180. ;
                longitude:standard_name = "longitude" ;
        float sun_zen_angle(time) ;
                sun_zen_angle:long_name = "solar zenith angle at the Earth\'s surface for the pixel center" ;
                sun_zen_angle:units = "degrees" ;
                sun_zen_angle:standard_name = "solar_zenith_angle" ;
        float satellite_zen_angle(time) ;
                satellite_zen_angle:long_name = "Metop zenith angle at the Earth\'s surface for the pixel center" ;
                satellite_zen_angle:units = "degrees" ;
                satellite_zen_angle:standard_name = "platform_zenith_angle" ;
        int orbit_number(time) ;
                orbit_number:long_name = "Metop orbit number" ;
        short scanline_number(time) ;
                scanline_number:long_name = "scanline number in the Metop orbit" ;
        short pixel_number(time) ;
                pixel_number:long_name = "pixel number in the current scanline" ;
                pixel_number:valid_range = 1., 120. ;
        short fov_number(time) ;
                fov_number:long_name = "field of view number in the 2 x 2 observation matrix" ;
                fov_number:valid_range = 1., 4. ;
        float surface_temperature(time) ;
surface_temperature:long_name = "temperature of the ground at surface level" ;
                surface_temperature:units = "K" ;
```

```
	float radiances_residual_mean(time) ;
		radiances_residual_mean:long_name = "mean of the residual of the fit (calculated-observed)" ;
		radiances_residual_mean:units = "W.cm-2.sr-1/cm-1" ;
	float radiances_residual_std(time) ;
		radiances_residual_std:long_name = "standard deviation of the residual of the fit (calculated-observed)" ;
		radiances_residual_std:units = "W.cm-2.sr-1/cm-1" ;
	float AVK(time, navkcols, navkrows) ;
		AVK:long_name = "averaging kernels for H2O and HDO (scaling factor)" ;
		AVK:block_h2o = "(1:13,1:13)" ;
		AVK:block_hdo = "(14:26,14:26)" ;
	float AVK_t2(time, navkcols, navkrows) ;
		AVK_t2:long_name = "averaging kernels for H2O and HDO type 2 (scaling factor)" ;
		AVK_t2:block_h2o_type2 = "(1:13,1:13)" ;
		AVK_t2:block_hdo_type2 = "(14:26,14:26)" ;
		AVK_t2:comments = "averaging kernels after a posteriori correction" ;
	float spectra_observed(time, nchannels) ;
		spectra_observed:long_name = "spectra observed" ;
		spectra_observed:units = "W.cm-2.sr-1/cm-1" ;
	float spectra_calculated(time, nchannels) ;
		spectra_calculated:long_name = "spectra calculated" ;
		spectra_calculated:units = "W.cm-2.sr-1/cm-1" ;
	float hdo_profile_t2(time, nlevels) ;
		hdo_profile_t2:long_name = "HDO profiles type 2" ;
		hdo_profile_t2:units = "mol/mol" ;
	float h2o_profile(time, nlevels) ;
		h2o_profile:long_name = "H2O profiles" ;
		h2o_profile:units = "mol/mol" ;
		h2o_profile:comments = "H2O profiles type 1" ;
	float h2o_profile_t2(time, nlevels) ;
		h2o_profile_t2:long_name = "H2O profiles type 2" ;
		h2o_profile_t2:units = "mol/mol" ;
	float dd_profile_t2(time, nlevels) ;
		dd_profile_t2:long_name = "deltaD profiles type 2" ;
		dd_profile_t2:units = "permil" ;
	float atmospheric_pressure_profile(time, nlevels) ;
		atmospheric_pressure_profile:long_name = "atmospheric pressure profile" ;
		atmospheric_pressure_profile:units = "hPa" ;
		atmospheric_pressure_profile:missing_value = -999. ;
		atmospheric_pressure_profile:comments = "diagnostic variable to be used up to 8 km only" ;
	float atmospheric_temperature_profile(time, nlevels) ;
		atmospheric_temperature_profile:long_name = "atmospheric temperature profile" ;
		atmospheric_temperature_profile:units = "K" ;
		atmospheric_temperature_profile:missing_value = -999. ;
		atmospheric_temperature_profile:comments = "diagnostic variable to be used up to 8 km only" ;
	float alt_asl(time, nlevels) ;
		alt_asl:long_name = "altitude above sea level" ;
		alt_asl:units = "km" ;
	float altitude_levels(nlevels) ;
		altitude_levels:long_name = "altitude" ;
		altitude_levels:units = "km" ;
	float wavenumbers(nchannels) ;
		wavenumbers:long_name = "wavenumbers" ;
		wavenumbers:units = "cm-1" ;
	float dofs_hdo_tot(time) ;
		dofs_hdo_tot:long_name = "degrees of freedom of hdo profiles" ;
	float dofs_hdo_ft(time) ;
		dofs_hdo_ft:long_name = "degrees of freedom for signal for the hdo profiles in the free troposphere (3-6
km)" ;

// global attributes:

:title = "IASI/Metop-A ULB-LATMOS deltaD (HDO/H2O) L2 products (vertical profile)" ;
```

```
		:institution = "ULB-LATMOS" ;
		:product_version = "201701.0" ;
		:history = "2019-01-28 19:30:38 - Product generated with retrieval code version 201701" ;
		:summary = "This dataset contains Level-2 deltaD, HDO and H2O  vertical profile product from IASI observations for the AM orbit." ;
		:source = "Eumetsat IASI Level-1C data (version 4 up to 20100518, version 5 from 20100518 to 20110929, version 6 from 20110929 to 20130808, version 7 from 20130808), Eumetsat IASI Level-2 data (version 4 up to 20100914, version 5 from 20100914 to 20140930, version 6 from 20140930, version 6.1 from 20150924, version 6.3 from 20170620), emissivities climatologies of Dan Zhou (from IASI data)" ;
		:references = "Reference to the deltaD retrieval: Lacour et al., Mid-tropospheric ˝˝D observations from IASI/MetOp at high spatial and temporal resolution, Atmos. Chem. Phys., 12, 10817-10832, https://doi.org/10.5194/acp-12-10817-2012, 2012. Lacour et al., Importance of the Saharan heat low in controlling the North Atlantic free tropospheric humidity budget deduced from IASI ˝˝D observations, Atmos. Chem. Phys., 17, 9645-9663, https://doi.org/10.5194/acp-17-9645-2017, 2017." ;
		:creator_name = "LATMOS-ULB" ;
		:contact_email = "contact form at http://iasi.aeris-data.fr/contact/" ;
		:data_policy = "Use of these data is free and open access. For substantial use (i.e. the results would have been different without the IASI dataset), please offer co-authorship and contact the principal investigators (Jean-Lionel Lacour, jlacour@hi.is; Cathy Clerbaux, Cathy.Clerbaux@latmos.ipsl.fr). For minor use (eg a plot), please notify the data owner, send a copy of the manuscript before publication, cite the proper references to the data as indicated in the references attribute, and acknowledge the AERIS data infrastructure and the data owner as follows: \"IASI is a joint mission of EUMETSAT and the Centre National d Etudes Spatiales (CNES, France). The authors acknowledge the AERIS data infrastructure for providing access to the IASI data in this study and ULB-LATMOS for the development of the retrieval algorithms.\"" ;
		:id = "IASI_METOPA_L2_deltaD_20090102_ULB-LATMOS_V201701.0.nc" ;
		:geospatial_lat_min = "-30.0" ;
		:geospatial_lat_max = "+30.0" ;
		:geospatial_latitude_units = "degrees_north" ;
		:geospatial_lon_min = "-180.0" ;
		:geospatial_lon_max = "+180.0" ;
		:geospatial_longitude_units = "degrees_east" ;
		:geospatial_vertical_min = "0.25" ;
		:geospatial_vertical_max = "11.5" ;
		:geospatial_vertical_units = "km" ;
		:time_coverage_start = "20090102T122825Z" ;
		:time_coverage_end = "20090102T224857Z" ;
		:comments = "This dataset contains IASI retrievals only for the AM orbit" ;
		:conventions = "CF-1.6" ;
		:standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Convention version 30, 3 December 2015" ;
		:keywords = "satellite,observation,atmosphere,deltaD,water vapor,H2O,HDO,level 2,profile,IASI,Metop-A" ;
		:keywords_vocabulary = "GCMD Science Keywords" ;
		:platform = "METOP-A" ;
		:sensor = "IASI" ;
		:spatial_resolution = "12km at nadir" ;
}
```

Retrieval methodology

To retrieve δD from IASI spectral radiances, we used the optimal estimation method, mainly following the approach proposed by Worden et al. (2006) and Schneider et al. (2006). It involves retrieving HDO and H2O with an a priori covariance matrix that represents the variability of the two species but also contains information on the correlations between them. The retrieval performed on a log scale allows better constraint of the solution and minimization of error on the δD profile (Worden et al., 2006; Schneider et al., 2006; Schneider and Hase, 2011). The line-by-line radiative transfer model software Atmosphit developed at the Université libre de Bruxelles (ULB) has been adapted to allow this HDO/H_2O correlated approach. Using correlations between log(HDO) and log(H_2O) helps to constrain the joint HDO/H_2O retrieval to a physically meaningful solution.

Considering the limited vertical sensitivity of retrieval

The error of a retrieval can be separated into 3 principal components:
(1) the smoothing error,
(2) the error due to uncertainties in model parameters, and
(3) the error due to the measurement noise.
The smoothing error is generally the largest error.

Following this, there are two ways to conduct an error analysis (EA), depending whether one considers the retrieval as an estimate of the true state with an error contribution due to smoothing (EA1), or as an estimate of the true state smoothed by the averaging kernels (EA2).

Averaging kernels type 1

The averaging kernels describe the sensitivity of the retrieval to the true variation of the state of the atmosphere. In the δD retrieval the averaging kernels are regrouped in 26*26 matrix which are composed of 4 sub-blocks. Each sub-block is a 13*13 matrix:

$$\boldsymbol{AVK} = \begin{matrix} \mathbf{A}_{\text{hh}} & \mathbf{A}_{\text{hd}} \\ \mathbf{A}_{\text{dh}} & \mathbf{A}_{\text{dd}} \end{matrix}$$

- $\mathbf{A}_{hh}$ corresponds to the sensitivity of the retrieved humidity profile to real variations of humidity
- $\mathbf{A}_{dd}$ corresponds to the sensitivity of the retrieved HDO profile to real variations of HDO
- $\mathbf{A}_{hd}$ corresponds to the sensitivity of the retrieved humidity profile to real variations of HDO
- $\mathbf{A}_{dh}$ corresponds to the sensitivity of the retrieved HDO profile to real variations of humidity

The corresponding δD profile is computed from variables hdo_profiles_t2 and h2o_profiles_t2:

$$\delta D = 1000 \left[\left(\frac{hdo_{profiles\_t2}}{h2o_{profiles\_t2}} \right) / 3.115e^{-4} - 1 \right]$$

Averaging kernels type 2

As there is more vertical information in the retrieved profile of humidity than HDO, there is a difference in vertical sensitivity between the humidity and δD profiles. For this reason, Wiegele et al., introduced a methodology to a posteriori correct the difference of vertical sensitivities in order to ensure that both humidity profile and δD profile are representative of the exact atmosphere. This a posteriori correction is provided in the netcdf files. When considering this approach, variables AVK_t2, h2o_profiles_t2 and dd_profiles_t2 must be used. The humidity profiles have been degraded to the vertical sensitivity of δD, and AVK_t2 (same structure than AVK) describe this sensitivity. The sub-blocks $\mathbf{A}_{hh}$ and Add are in that case identical. **For simplicity it is recommended to use this type 2 product.**

Error analysis 2 (EA2): considering the retrieval as an estimate of the true state smoothed by the averaging kernels

This is the ideal approach. In comparisons model – data, this approach should be used. The error to consider in that case is the error due to uncertainties in model parameters (2) and the error due to the measurement noise (3). The resulting error has been estimated to 38 permil (between 3 and 6 km) on an individual basis. When considering several measurements, this error which is random can be reduced by a factor sqrt(n) with n being the number of measurements used in the averaging.

To compare model to data using this approach it is necessary to degrade the vertical information contained in model profiles to the limited sensitivity of the retrieval. This can be easily achieved with the averaging kernels matrix:

For the humidity profile:
First the model profiles need to be interpolated at IASI vertical grid. Then the interpolated q (humidity) profile can be smoothed:

$$\delta D = 1000\left[\left(\frac{hdo_{profiles\_t2}}{h2o_{profiles\_t2}}\right)/3.115e^{-4} - 1\right]$$

qsm=smoothed profile of q, Ahh=Averaging kernels corresponding to the retrieval of humidity (AVK(1:13,1:13)), q=model humidity profile interpolated at the retrieval levels, In= identity matrix, qp= a priori specific humidity profile used in the retrieval.

The same approach applies for an optimal use of humidity and δD profiles (type 2). In that case, the matrix AVK_t2 must be used.

Error analysis 1 (EA1): considering the retrieval as an estimate of the true state with an error contribution due to smoothing

If δD retrievals are used in other context that model-data comparison or when the smoothing is not possible, it is important to keep in mind the limited information contained in the retrieved profile. For example, if δD observations at 3.5 km are used in parallel to airmass trajectory analysis it is important to consider the trajectory of the airmasses arriving between 2 and 5 km and not only at 3.5 km.