MesosphEO WP 4.1: Preparatory works

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1. Introduction

This document defines the netCDF formats to be used for Level 2 and Level 3 products in the ESA's MesosphEO project.

2. Selection of format

The files will be made for netCDF4. Variable naming should follow as much as possible the available Climate and Forecast standard (see http://cfconventions.org). This standard is not targeted for satellite data and does not include all the variable names needed in the data files of this project. An important application of this standard is the O3-CCI format (Sofieva et al., 2013 and http://www.esa-ozone-cci.org). It is proposed to follow this example in the MesosphEO-files.

3. User guidance for data

All data collections should accompany a short Read Me document. A user should easily find how to select the best quality of data for his/her purpose. An estimation for data quality can be a quality flag or data with questionable quality can be excluded from the data set.

4. Level 2 data format

These files are data from individual measurements by the instrument. The data variables can be collected to six categories:

1. Common geolocation of measurement
   - -time (from 1.1.1900)
   - -latitude (-90°... 90º)
   - -longitude (-180°... 80°)
   - -altitude or pressure
   - -solar zenith at measurement altitude
   - -solar azimuth (if relevant)
2. Retrieval results
   - -concentration
   - -concentration error
   - -vertical resolution

   Note: concentration will be provided in the unit that is "natural" to the instrument. The concentration can also be given in an additional unit if needed. In this case the transformation factor or field must also be included in the product or documented.

3. Specific data for selection (if relevant). Examples:
   - -local time
   - -quality flags

- chi2 values
-target identification
- mpv values
-magnetic coordinates
-equivalent latitude
-valid altitude ranges

4. Satellite specific data. Examples:
-orbit number
-solar zenith angle at satellite
-South Atlantic Anomaly flag
-beta angle
5. Used a priori data (if relevant). Examples:
-ECMWF
-MERRA
-MSIS
6. Global attributes
-source file identification
-instrument name
-platform name
-source data version
-data version
-data creation date
-project name
-institute responsible
-file created by email
-data filtering applied

In netCDF-4 groups could be used to separate these different data. For short number of variables this is not needed.

An example GOMOS O3-CCI file from V. Sofieva:

Table 1. Parameters in the GOMOS HARMOZ_PRS files.

Parameter and unit	*Dimensions*	*Description*
time (days since 1900-01-01 00:00:00)	N_{prof}×1	The parameter to index the profiles
pressure (hPa)	N_{alt}×1	The vertical coordinate, air pressure
altitude (km)	$N_{alt} \times N_{prof}$	The geometric altitude above the mean sea-level
latitude (degree_north)	N_{prof}×1	Latitude of each profile
longitude (degree_east)	N_{prof}×1	Longitude of each profile
ozone_concentration (mol/m^3)	$N_{alt} \times N_{prof}$	Mole concentration or number of moles per unit volume (molarity) of ozone. Multiplication factor to convert to molecules/cm^{3}is 6.022140857E+17
ozone_concentration_standard_error (mol/m^3)	$N_{alt} \times N_{prof}$	Uncertainty (random error) associated with the ozone profiles. Multiplication factor to convert to molecules/cm^{3}is 6.022140857E+17.
vertical_resolution (km)	N_{alt}×1	FWHM of the averaging kernel
air_temperature (K)	$N_{alt} \times N_{prof}$	Temperature profiles at the locations of measurements, for conversion from concentration to mixing ratio
orbit_number	N_{prof}×1	Envisat orbit number
star_number	N_{prof}×1	Star number in GOMOS catalogue
star_magnitude	N_{prof}×1	Star visual magnitude
star_temperature (K)	N_{prof}×1	Star effective temperature
obliquity (deg)	N_{prof}×1	Obliquity of occultation: the angle between the orbital plane and the line of sight
sza (deg)	N_{prof}×1	solar zenith angle at tangent point
chi2	$N_{alt} \times N_{prof}$	Profiles of normalized χ^2- statistics. Usually close to 1. Large values indicate problems with retrievals
illumination_condition_flag	N_{prof}×1	0-full dark, 3-straylight, 2- twilight, 4- straylight&twilight.
SAA_flag	N_{prof}×1	The indicator showing that the data might be affected by the Southern Atlantic Anomaly (cosmic rays); 0- no, 1- yes

5. Level 2 vertically gridded data format

These files are data from individual measurements by the instrument and collected on to a vertical coordinate grid where the vertical coordinate can be geometrical altitude or pressure. The geometrical altitude grid is usually with 1 km spacing. An example of the pressure grid is the following used in the O3-CCI project (unit hPa):

450, 400, 350, 300, 250, 200, 170, 150, 130, 115, 100, 90, 80, 70, 50, 40, 30, 20, 15, 10, 7, 5, 4, 3, 2, 1, 1.5, 1, 0.7, 0.5, 0.4, 0.3, 0.2, 0.15, 0.1, 0.07, 0.05, 0.04, 0.03, 0.02, 0.015, 0.01, 0.007, 0.005, 0.004, 0.003, 0.002, 0.0015, 0.001, 0.0007, 0.0005, 0.0004, 0.0003, 0.0002, 0.00015, 0.0001.

A stratospheric subset of this grid is used in SPARC-DI project.

The data format is based on the format presented in Sec. 4 with the following added variables:

-altitude or pressure grid (this replaces altitude or pressure variable)

-gridding method

6. Level 3 individual instrument data format

These files are data from individual measurements by the instrument and collected on to a vertical coordinate-latitude-time grid where the vertical coordinate can be geometrical altitude or pressure. The agreed grid is 10 degrees in latitude from -90° to 90°, and monthly in time. The geometrical altitude grid is with 1 km spacing. The pressure grid is the same used in the O3-CCI (see Sec. 5),

The data variables can be collected to five categories (with examples of possible variables):

1. Grids
   - -vertical grid
   - -mid-points of the latitude cells
   - -mid-points of the time cells (i.e. mid-month)
2. Gridding results
   - -average concentration in latitude-time cells
   - -estimated error of the average
   - -std
   - -quartiles
   - -number of measurements in latitude-time cells
3. Statistical methods
   - -estimating methods in the latitude-time space (mean, median, weighted mean etc.)
   - -average latitude of measurements in latitude-time cells
   - -average time of measurements in latitude-time cells
   - - possible measures to characterise the distribution inside latitude-time cells
   - -interpolation method of individual profiles to the vertical grid
4. Data selection
   - -data filtering applied
5. Global attributes
   - -source file identification
   - -instrument name
   - -platform name
   - -source data version
   - -data version
   - -data creation date
   - -project name
   - -institute responsible
   - -file created by email
   - -data filtering applied

7. Level 3 multi-instrument data format

These data are like the ones in Sec. 6, but the value in a latitude-time cell is calculated as an average of data from several instruments. There are several methods how to combine data from several data sources and the method selected must be specified in the new data set. Added variables in the multi-instrument data are:

-combination method (Examples: an average over all measurements, average of individual instrument measurement populations)
-number of measurements in individual instrument measurement populations
-estimated error of the combined value
-unique identification to the individual instrument data

8. Repository

Level 2 original data will be preserved and maintained by the institute/university that has produced the data set. Finnish Meteorological Institute (FMI) will maintain a link list of the data repositories on the MesosphEO-project's web-page. FMI will preserve the new data sets created in the MesosphEO project and make them available by the project's web-page.

9. References

Kyrölä et al., ALGOM WP5: GOMOS User Friendly Products: Read Me-document, FMI-ALGOM-TN-005, 2016

Sofieva, V. F. et al. (2013), Harmonized dataset of ozone profiles from satellite limb and occultation measurements, Earth Syst. Sci. Data, 5(2), 349–363, doi:10.5194/essd-5-349-2013. [online]
Available from: http://www.earth-syst sci-data.net/5/349/2013/

ESA MesosphEO project plan, version 1.5, 2016