Semi-monthly mean ozone profiles

Data description and user manual

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1. Introduction

This technical note describes semi-monthly mean ozone profiles (from individual instruments and merged) using the Envisat limb instruments (GOMOS, MIPAS, SCIAMACHY) and the ESA Third Party Mission instruments (OSIRIS, SMR, and ACE-FTS). This dataset is targeted mainly for climate modeling and climate research.

The dataset includes mean ozone profiles in 10° latitude × 20° longitude zones, twice per month, as well as the parameters, which characterize the uncertainty of the merged profiles. The data cover the years 2007-2008 (in Phase 1 of the ozone-CCI project). The ozone profiles are presented on ozone-CCI pressure grid (Sofieva et al., 2013a) from 250 hPa to 1 hPa.

The general approach of computing semi-monthly mean data is the same as for creating monthly zonal mean ozone profiles (Sofieva, 2013bc): first semi-monthly mean (SMM) data from individual instruments are created, and then the weighted mean of SMM data is used as a merged semi-monthly mean (MSMM) ozone profiles.

This Technical Note is organized as follows. Section 2 shortly described the computing and characterization of semi-monthly mean ozone profiles from individual instruments. Section 3 is dedicated to data merging. Section 4 describes the structure of netcdf files.

2. Semi-monthly data from individual instruments (SMM)

For the SMM dataset, ozone profiles from individual HARMOZ datasets (Sofieva et al., 2013a; Rahpoe and Lloyd, 2013) are averaged in 10° latitude × 20° longitude zones, twice per month. The data averaging and characterization is performed in the same way as for monthly zonal mean data (Sofieva et al., 2013b), i.e., via computing the mean of ozone profiles. Examples of the created ozone fields are presented in Figures 1 and 2. Despite overall agreement, the ozone distributions from different instruments have own peculiarities. In particular, wave 1 structure at 50°-60°N is observed for all instruments, but the amplitude and the phase are slightly different. Noisiness of SMR data is observed also in semi-monthly mean data.

SMM ozone profiles are characterized by:

- the standard error of the mean:

$$\sigma^2_{mean} = \frac{s^2}{N}, \quad (1)$$

where $s^2 = \left\langle (x_k - \overline{x})^2 \right\rangle$ is sample variance and *N* is the number of measurements;

- inhomogeneity in latitude, longitude and in time:

$$H = \tfrac{1}{2}(A + (1 - E)), \qquad (2)$$

where *A* and *E* are anisotropy and entropy, respectively.

Figure 3 illustrates the inhomogeneity measures in latitude, longitude, and in time for 1- 16 January 2008, at 15 hPa pressure level (~30 km). As observed in Figure 3, the inhomogeneity in longitude is usually small practically for all sensors.

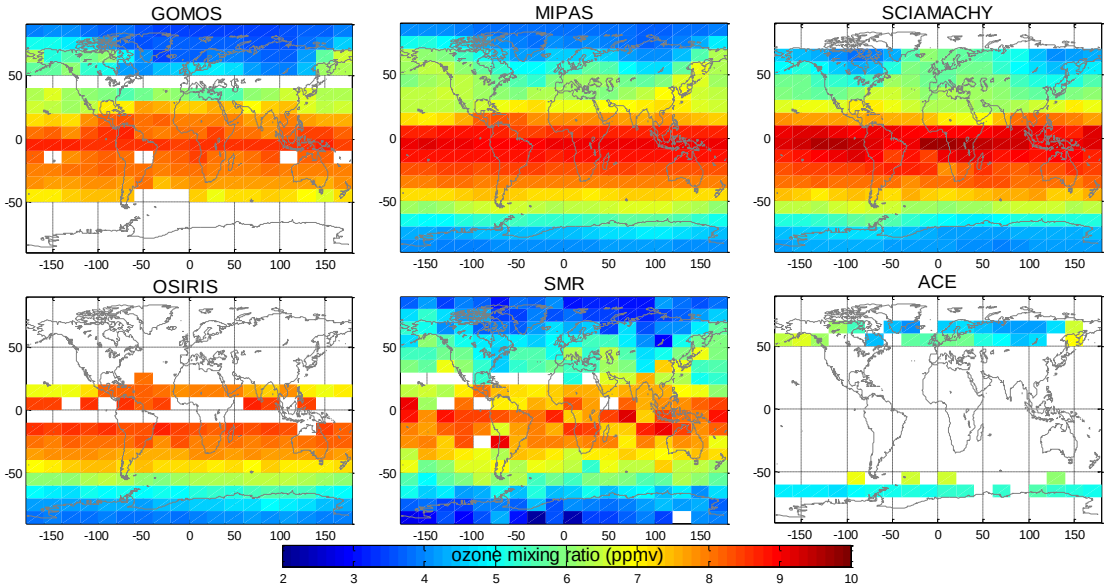

Figure 1. Ozone mixing ratio (ppmv) at 15 hPa (~30 km) for 1-16 January 2008.

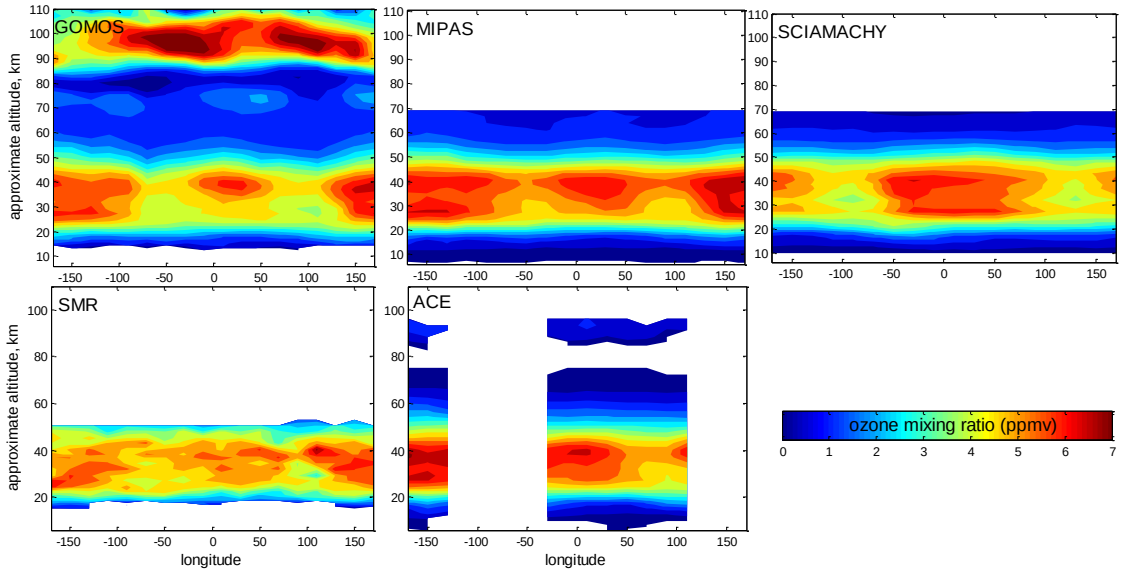

Figure 2. Ozone mixing ratio (ppmv) profiles at latitudes 50°-60° N as a function of longitude, for 1-16 January 2008.

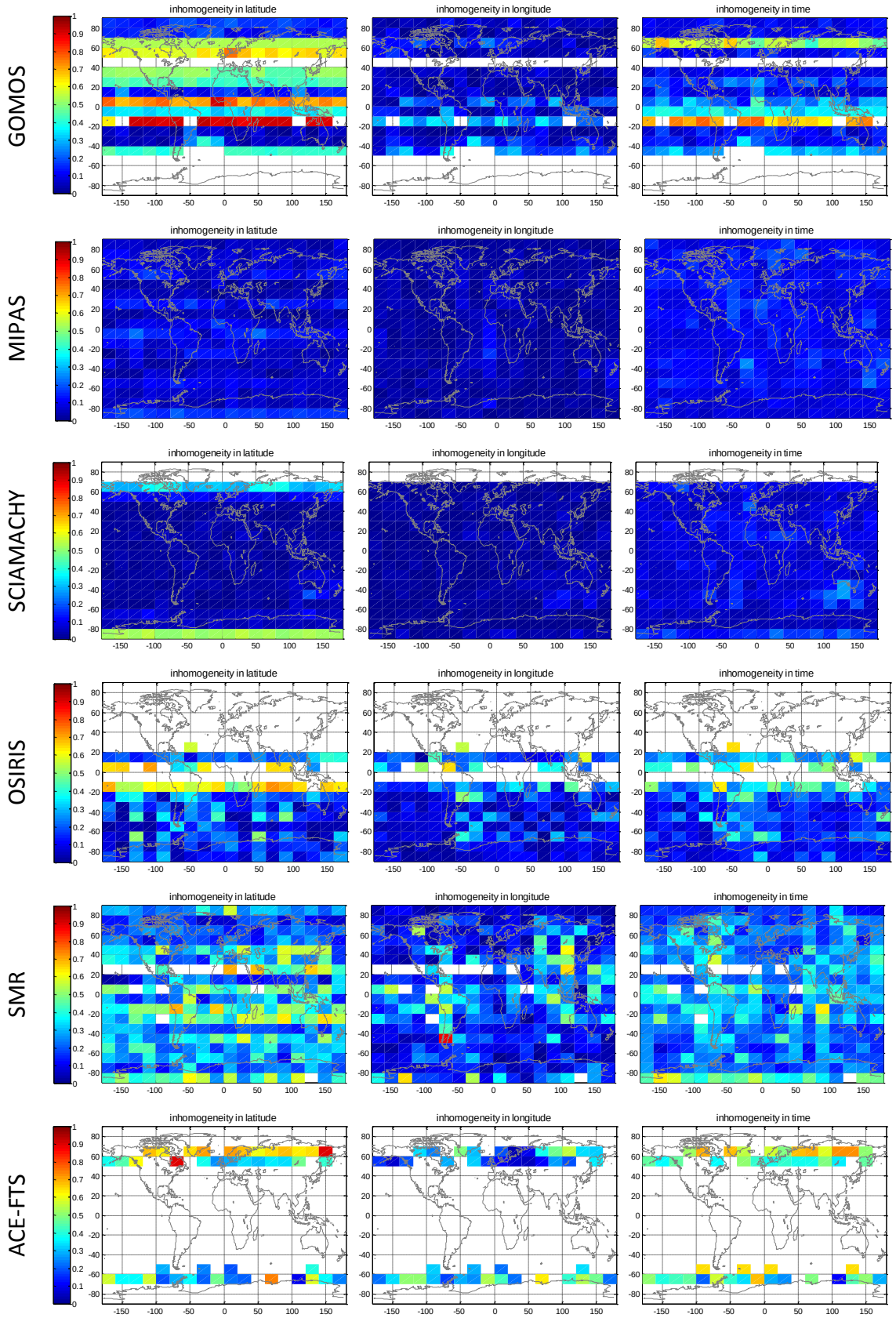

Figure 3. Inhomogeneity measures in latitude, in longitude and in time at 15 hPa(~30 km) for 1-16 January 2008.

3. Merged semi-monthly mean ozone profiles (MSMM)

The data merging is performed in full analogy with creating monthly zonal mean data. Below we outline main steps of data processing.

Semi-monthly merged dataset is created in the altitude range from ~10 km up to ~ 50 km (250 hPa – 1 hPa), in order to avoid significant diurnal variations at upper altitudes. For each instrument, the uncertainty of semi-monthly mean values is:

$$\sigma^2 = \sigma^2_{mean} + \sigma^2_{sampling} \tag{3}$$

The first term, σ^2_{mean}, is the standard error of the mean, Eq (1). The second term, $\sigma^2_{sampling}$, is the sampling uncertainty, which is related to potentially non-uniform sampling by measurements in space and in time. For its characterization, we use a relation [Sofieva et al., 2012]:

$$\sigma_{sampling} = \frac{1}{2}\left(H_{lat} + H_{time}\right)\cdot\sigma_{nat}\,, \tag{4}$$

where H_{lat} and H_{time} are inhomogeneity measures in latitude and in time, respectively, and σ_{nat} is the profile of natural variability taken from LLM climatology [*McPeters et al.*, 2007], for each month and each latitude bin. In principle, ozone variability in 10°×20° latitude-longitude bands should be used instead of zonal variability in (4). However, such information is not available at the moment. After creating longitude-resolved climatology of ozone variability, characterization of sampling error can be improved. Analogously, inhomogeneity in longitude can also be included in this future advanced characterization.

Uncertainties of the mean values σ_{mean}, sampling error $\sigma_{sampling}$ and total error σ (Eq.(3)) of the instrument-based zonal mean data in 1-16 January 2008 at 15 hPa level are shown in Figure 4.

The merged semi-monthly zonal mean is computed in each latitude-longitude bin as the weighted mean of the zonal mean datasets from individual instruments, with the weights α_i that are inversely proportional to uncertainties σ_i^2 (Eq.(3)):

$$\begin{aligned} \rho_{merged} &= \sum_{i=1}^{N_{instru}} \alpha_i \rho_i \\ \alpha_i &= \frac{1/\sigma_i^2}{\sum 1/\sigma_i^2} \end{aligned} \tag{5}$$

The merged zonal mean ozone data for 1-16 January 2008 is shown in Figure 5.

The associated uncertainty of the merged dataset will be defined by:

$$\sigma^2_{merged} = \frac{1}{\sum_{i=1}^{N_{instru}} 1/\sigma_i^2} \cdot \frac{1}{(N_{insru}-1)} \sum_{i=1}^{N_{instru}} \frac{(\rho_i - \rho_{merged})^2}{\sigma_i^2}\,. \tag{6}$$

The first factor in (6), $\frac{1}{\sum_{i=1}^{N_{instru}} 1/\sigma_i^2} = \sigma^2_{wmean}$, is the uncertainty of the weighted mean provided the uncertainties σ_i are the only source of variations in ozone. The second factor

in Eq. (6) takes into account variability between the datasets. The uncertainties σ_{merged} for the ozone distributions of Figure 5 are illustrated in Figure 6.

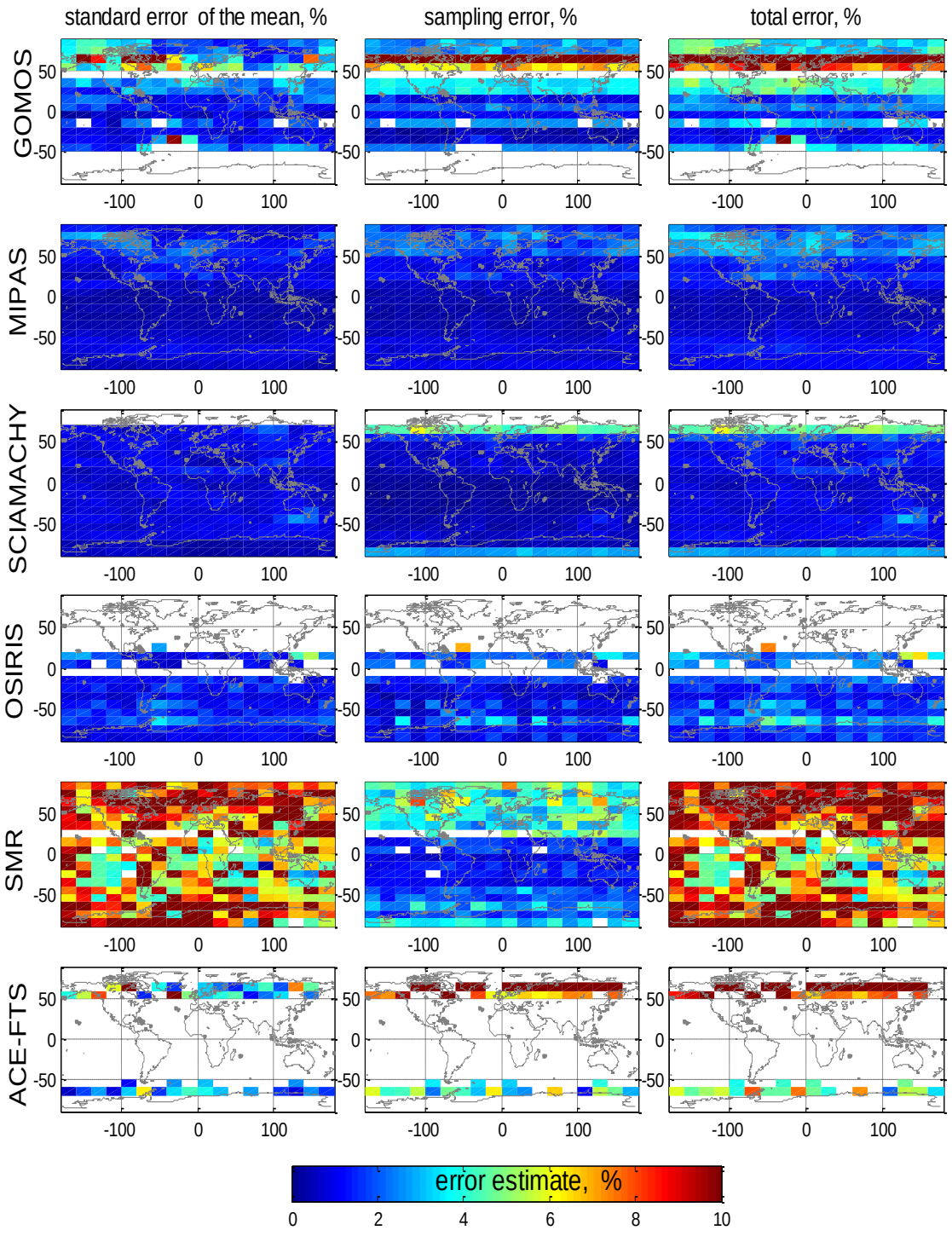

Figure 4 Uncertainty of the mean values, sampling error $\sigma_{sampling}$ and total error of the instrument-based semi-monthly mean data at 15 hPa (~30 km), for 1- 16 January 2008. All uncertainties are presented in %.

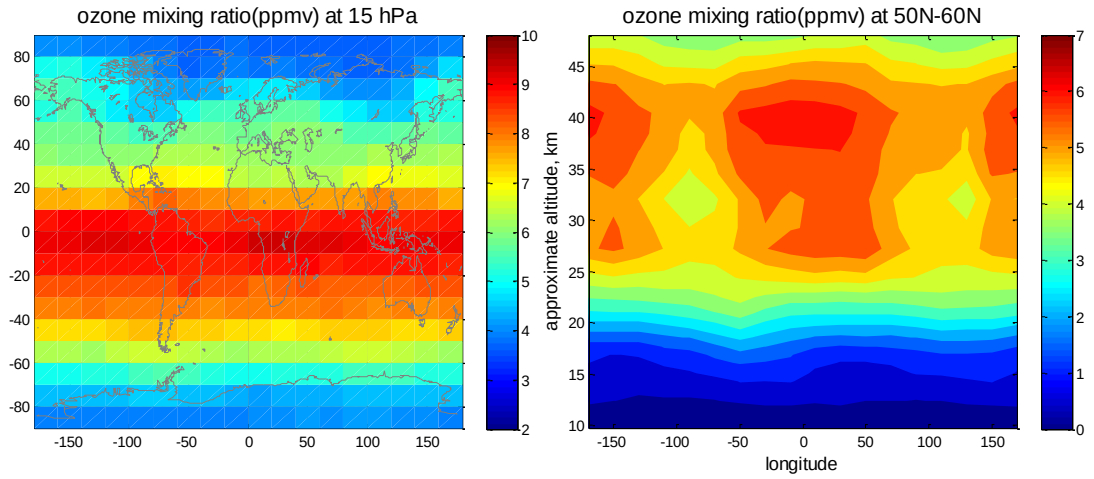

Figure 5. (a) Longitude-latitude section at 15 hPa (~30 km) and (b) longitude-altitude section at 50°-60°N from the merged semi-monthly mean ozone field for 1-16 January 2008.

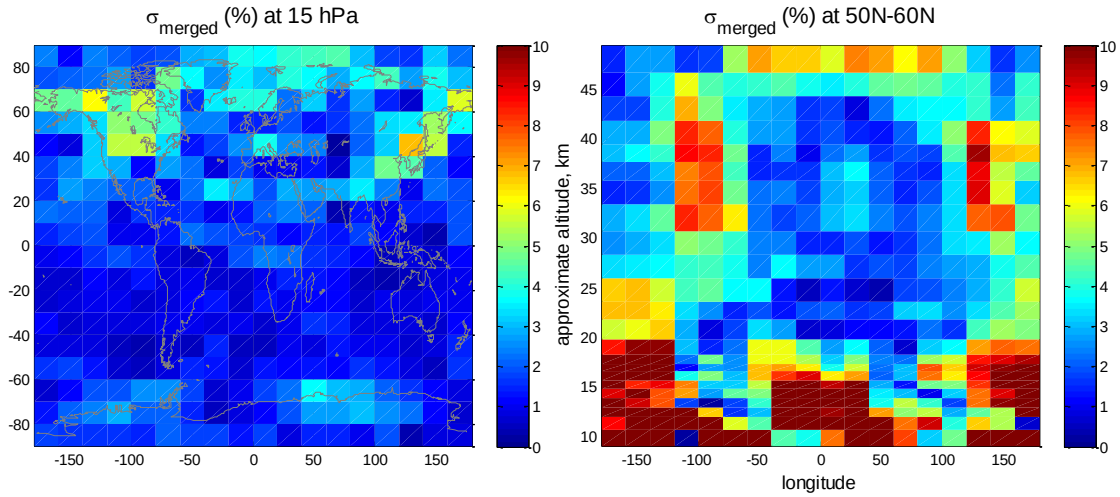

Figure 6. Uncertainties (in %) associated with the merged semi-monthly mean profiles, for the distributions shown in Figure 5.

4. The data format

The merged semi-monthly mean ozone profiles are structured into yearly netcdf files with self-explanatory names. For example, the file "ESACCI-OZONE-L3-LP-SMM-2008-fv0002.nc" contains the semi-monthly mean ozone profiles for January 2008. In addition to the variables of the merged data, the profiles from individual instruments with their uncertainty parameters are also included (for the altitude range 250-1 hPa used in data merging). The variables included into netcdf files are collected in Table 1. An example of the full structure of the netcdf file is presented in Appendix A.

References

McPeters, R. D., G. J. Labow, and J. A. Logan (2007), Ozone climatological profiles for satellite retrieval algorithms, *J. Geophys. Res.*, *112*(D5), D05308, doi:10.1029/2005JD006823.

Rahpoe, N., and N. D. Lloyd (2013), *Ozone Limb Level 2 Harmonized Single Instrument Document*

Sofieva V.F., Kalakoski N., and Päivärinta S.-M. (2012): Sampling error of satellite instruments, Technical Note.

Sofieva et al., (2013a): Harmonized dataset of ozone profiles from ESA Envisat and Third Party Missions limb measurements, Technical Note.

Sofieva et al., (2013b): Instrument-based monthly zonal mean ozone profiles, Technical Note, 15 Apr 2013.

Sofieva et al., (2013c): Merged monthly zonal mean ozone profiles, Technical Note, 18 Apr 2013.

Table 1. The variables in MSMM netcdf files. N_{alt} is number of pressure levels, N_{lat} and N_{lon} are numbers of latitude and longitude bins, respectively, N_{time} is number if temporal intervals and N_{instru} =6 is number of instruments.

	Parameter and unit	*Dimensions*	*Description*
General parameters	air pressure (hPa)	$N_{alt}\times 1$	The vertical coordinate
	approximate_altitude (km)	$N_{alt}\times 1$	Approximate altitude at pressure levels computed as $z = 16\log_{10}(1013/P)$, P is pressure in hPa
	latitude_centers (degree_north)	$N_{lat}\times 1$	Centers of latitude bins: -85°: 10°:85°
	longitude_centers (degree_east)	$N_{lon}\times 1$	Centers of longitude bins: -170°:20°:170°
	time	$N_{time}\times 1$ (24×1)	Central date for each half of month, expressed as days since
	instruments	$N_{instru}\times 1$	A dimension for individual datasets, instrument order 1-GOMOS, 2-MIPAS, 3-SCIAMACHY, 4-OSIRIS, 5-ACE-FTS , 6-SMR
Merged data	merged_ozone_vmr	$N_{lat}\times N_{lon}\times N_{alt}\times N_{time}$	Merged semi-monthly zonal mean ozone mixing ratio vertical profiles
	merged_ozone_concentration (mol/cm^3)	$N_{lat}\times N_{lon}\times N_{alt}\times N_{time}$	Vertical profiles of merged semi-monthly zonal mean ozone mole concentration. Number density (cm^{-3}) is acquired by multiplying the variable with Avogadro constant N_A=6.02214×10^{23} mol^{-1}
	uncertainty_of_ merged_ozone (%)	$N_{lat}\times N_{lon}\times N_{alt}\times N_{time}$	Uncertainty σ_{merged} of the merged data, Eq.(6)
Individual datasets	ozone_vmr	$N_{lat}\times N_{lon}\times N_{alt}\times N_{time}$	Semi-monthly zonal mean ozone mixing ratio vertical profiles for individual instruments
	ozone_mole_concentration (mol/cm^3)	$N_{instru}\times N_{lat}\times N_{lon}\times N_{alt}\times N_{time}$	Semi-monthly zonal mean ozone mole concentration vertical profiles for individual instruments.
	standard_error_of_ the_mean (%)	$N_{instru}\times N_{lat}\times N_{lon}\times N_{alt}\times N_{time}$	Uncertainty of the semi-monthly zonal mean for individual datasets, σ_{mean}, Eq. (1)
	sampling_error (%)	$N_{instru}\times N_{lat}\times N_{lon}\times N_{alt}\times N_{time}$	Sampling error $\sigma_{sampling}$ for individual datasets characterized using (4).
	total_ error (%)	$N_{time}\times N_{lat}\times N_{lon}\times N_{alt}\times N_{instru}$	Total uncertainty of semi-monthly zonal mean data from individual instruments, see Eq.(3)
	inhomogeneity_in_ longitude	$N_{instru}\times N_{lat}\times N_{lon}\times N_{alt}\times N_{time}$	Inhomogeneity measure in latitude, Eq.(4)
	inhomogeneity_in_ latitude	$N_{instru}\times N_{lat}\times N_{lon}\times N_{alt}\times N_{time}$	Inhomogeneity measure in latitude, Eq.(4)
	inhomogeneity_in_ time	$N_{instru}\times N_{lat}\times N_{lon}\times N_{alt}\times N_{time}$	Inhomogeneity measure in time, Eq.(4)

Appendix A: The structure of the MSMM netcdf file

The example of the structure of netcdf file is presented January 2008.

```
Format:
        netcdf4_classic
Global Attributes:
        title                 = 'ESA CCI ozone  merged semi-monthly  mean profiles '
        summary               = 'merged semi-monthly mean ozone profiles(MSMM) in 10-deg latitude zones
and data uncertainty characterization'
        comment               = 'semi-monthly  mean from individual sensors are also presented. Definitions
of parameters and data processing are described in the dedicated Technical Note'
        year                  = '2008'
        number_of_pressure_levels = '23'
        number_of_latitude_bins   = '18'
        number_of_longitude_bins  = '18'
        number_of_temporal_bins   = '24'
        geospatial_lat_resolution = '10 deg '
        geospatial_lat_min        = '-90 deg'
        geospatial_lat_max        = '90 deg'
        geospatial_lon_resolution = '20 deg '
        geospatial_lon_min        = '-180 deg'
        geospatial_lon_max        = '180 deg'
        geospatial_vertical_min   = ' 250 hPa'
        geospatial_vertical_max   = '1 hPa'
        value_for_nodata          = 'NaN'
        date_created              = '20130517T111336'
        creator_name              = 'Viktoria Sofieva'
        creator_email             = 'viktoria.sofieva@fmi.fi'
        address                   = 'P.O.Box 503, 00101 Helsinki, Finland'
        naming_authority          = 'FMI - Finnish Meteorological Institute'
        Conventions               = 'CF-1.5'
        standard_name_vocabulary  = 'NetCDF Climate and Forecast(CF) Metadata Convention version 18'
        license                   = 'ozone_cci guidelines'
        restriction               = 'Restricted under the use of ozone cci guidelines'
        file_version              = 'fv0001'
        tracking_id               = '90579'
Dimensions:
        air_pressure      = 23
        latitude_centers  = 18
        longitude_centers = 18
        time              = 24
        instruments       = 6
Variables:
   air_pressure
        Size:       23x1
        Dimensions: air_pressure
        Datatype:   double
        Attributes:
                units       = 'hPa'
                standard_name = 'air_pressure'
   latitude_centers
        Size:       18x1
        Dimensions: latitude_centers
        Datatype:   double
        Attributes:
```

```
            units       = 'degree_north'
            standard_name = 'latitude'
            long_name     = 'centers of latitude bins'
    longitude_centers
        Size:      18x1
        Dimensions: longitude_centers
        Datatype:   double
        Attributes:
            units       = 'degree_east'
            standard_name = 'longitude'
            long_name     = 'centers of longitude bins'
    time
        Size:      24x1
        Dimensions: time
        Datatype:   double
        Attributes:
            units       = 'days since 1900-01-01 00:00:0.0'
            standard_name = 'time'
            calendar      = 'standard'
    approximate_altitude
        Size:      23x1
        Dimensions: air_pressure
        Datatype:   double
        Attributes:
            units       = 'km'
            standard_name = 'altitude'
            long_name     = 'approximate altitude corresponding to pressure levels'
    instruments
        Size:      6x1
        Dimensions: instruments
        Datatype:   int16
        Attributes:
            units     = '1'
            long_name = 'index of instruments: 1-GOMOS, 2-MIPAS, 3-SCIAMACHY, 4-OSIRIS, 5-ACE-FTS,
6-SMR'
    merged_ozone_vmr
        Size:      18x18x23x24
        Dimensions: latitude_centers,longitude_centers,air_pressure,time
        Datatype:   double
        Attributes:
            units       = '1'
            standard_name = 'mole_fraction_of_ozone_in_air'
            long_name     = 'merged semi-monthly mean ozone mixing ratio'
    merged_ozone_concentration
        Size:      18x18x23x24
        Dimensions: latitude_centers,longitude_centers,air_pressure,time
        Datatype:   double
        Attributes:
            units       = 'mol cm-3'
            standard_name = 'mole_concentration_of_ozone_in_air'
            long_name     = 'merged semi-monthly mean ozone mole concentration'
    uncertainty_of_merged_ozone
        Size:      18x18x23x24
        Dimensions: latitude_centers,longitude_centers,air_pressure,time
        Datatype:   double
        Attributes:
            units     = '%'
```

long_name = 'total uncertainty of merged ozone profiles'
ozone_mole_concentration
Size: 6x18x18x23x24
Dimensions: instruments,latitude_centers,longitude_centers,air_pressure,time
Datatype: double
Attributes:
units = 'mol cm-3'
standard_name = 'mole_concentration_of_ozone_in_air'
long_name = 'semi-monthly mean concentrations from individual instruments'
ozone_vmr
Size: 6x18x18x23x24
Dimensions: instruments,latitude_centers,longitude_centers,air_pressure,time
Datatype: double
Attributes:
units = '1'
standard_name = 'mole_fraction_of_ozone_in_air'
long_name = ' semi-monthly mean mixing ratio from individual instruments'
standard_error_of_the_mean
Size: 6x18x18x23x24
Dimensions: instruments,latitude_centers,longitude_centers,air_pressure,time
Datatype: double
Attributes:
units = '%'
long_name = 'standard error of the mean for individual instruments'
sampling_error
Size: 6x18x18x23x24
Dimensions: instruments,latitude_centers,longitude_centers,air_pressure,time
Datatype: double
Attributes:
units = '%'
long_name = 'sampling error for individual instruments'
total_error
Size: 6x18x18x23x24
Dimensions: instruments,latitude_centers,longitude_centers,air_pressure,time
Datatype: double
Attributes:
units = '%'
long_name = 'total uncertainty of semi-monthly mean data for individual instruments'
inhomogeneity_in_time
Size: 6x18x18x23x24
Dimensions: instruments,latitude_centers,longitude_centers,air_pressure,time
Datatype: double
Attributes:
units = '1'
long_name = 'inhomogeneity measure in time'
inhomogeneity_in_latitude
Size: 6x18x18x23x24
Dimensions: instruments,latitude_centers,longitude_centers,air_pressure,time
Datatype: double
Attributes:
units = '1'
long_name = 'inhomogeneity measure in latitude'
inhomogeneity_in_longitude
Size: 6x18x18x23x24
Dimensions: instruments,latitude_centers,longitude_centers,air_pressure,time
Datatype: double
Attributes:

units = '1'
long_name = 'inhomogeneity measure in longitude'

Acronyms

ESA	European Space Agency
ozone-CCI	Ozone Climate Change Initiative
GOMOS	Global Ozone Monitoring by Occultation of Stars
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
SCIAMACHY	Scanning Imaging Spectrometer for Atmospheric Chartography
OSIRIS	Optical Spectrograph and InfraRed Imaging System
SMR	Sub-Millimeter Radiometer
ACE-FTS	Atmospheric Chemistry Experiment – Fourier Transform Spectrometer
SMM	Semi-monthly Mean
MSMM	Merged Semi-monthly Mean