SCIAMACHY WFM-DOAS (WFMD) methane, carbon monoxide, and carbon dioxide columns: Algorithm description and product specification

Valid for:

SCIAMACHY WFM-DOAS

Product	**Version**
Carbon monoxide vertical column (CO)	WFMD v0.6
Methane dry-air column averaged mole fraction (XCH_4)	WFMD v1.0
CO_2 dry-air column averaged mole fraction (XCO_2)	WFMD v1.0

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1 Purpose of document

The purpose of this document is to provide the algorithm description and product specification for the following scientific data products retrieved from the near-infrared / short wave infrared (NIR/SWIR) nadir spectra of the SCIAMACHY instrument onboard ENVISAT:

Product	Details	Algorithm	Current version
CO column	Vertical column of carbon monoxide in molecules/cm^2	WFM-DOAS	0.6
XCH4	XCH4 is the dry air column averaged mole fraction of methane in ppb (parts per billion)	WFM-DOAS	1.0
XCO2	XCO2 is the dry air column averaged mole fraction of carbon dioxide in ppm (parts per million)	WFM-DOAS	1.0

For all three products three years of SCIAMACHY data have been processed: 2003-2005.

All available information about our data products has been compiled on the SCIAMACHY WFM-DOAS web page, which is continuously updated:
http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/index.html
On this web page the following is available: PDF files of papers, poster, technical reports, etc., averaging kernels and a-priori profiles (ASCII files), sample data product files, global maps, data access information, point of contact information, etc.

The three data products are treated independently from each other in this document. If a reader is interested in only one particular data product he/she only needs to read the sections related to this product. This means, however, that this document contains redundant parts, as certain information is basically identical for two or all three data products.

The main reference for the CO WFMDv0.6 product is Buchwitz et al., 2007a. The latest peer-reviewed publication related to our CO WFMDv0.6 product is Khlystova et al., 2009.

Publications discussing in detail the XCO2 WFMDv1.0 products are Buchwitz et al., 2007b, and Schneising et al., 2008.

The main reference for the XCH4 WFMDv1.0 product is Schneising et al., 2009.

2 Algorithm description

2.1 Carbon monoxide retrieval algorithm

Algorithm: WFM-DOAS v0.6.

Most relevant reference: Buchwitz et al., 2007a.

Validation: Dils et al., 2006b, and Buchwitz et al., 2007a.

The algorithm is described in Buchwitz et al., 2007a. Here we limit ourselves to a short overview. For details including a full list of references please see Buchwitz et al., 2007a.

2.1.1 Major changes compared to previous version

General information about previous version:

- Algorithm previous version: WFM-DOAS v0.5.
- Most relevant reference: Buchwitz et al., 2006a.
- Validation: Dils et al., 2006a.

Major changes compared to previous version (details see Buchwitz et al., 2007a):

- Use of spectra with improved calibration: Level 1 version 5 (with nominal calibration) instead of (dark signal patched) version 4.
- Use of improved spectroscopy: HITRAN 2004 instead of HITRAN 2000/2001.
- Use of a newly generated static dead/bad detector pixel mask optimised for the time period 2003-2005.
- Processing of a longer time series: 2003-2005 instead of 2003.
- Optimisation of criteria, which determine a successful measurement (Quality flag).
- Slight modification of spectral fitting window (the version 0.6 fitting window located in SCIAMACHY channel 8 is: 2324.4-2335.0 nm; the version 0.5 window was: 2324.0-2335.0 nm).

2.1.2 Forward model

The forward model is the radiative transfer model SCIATRAN version 1.2 (Buchwitz et al., 2000a). SCIATRAN takes multiple scattering fully into account. SCIATRAN solves the radiative transfer equation for pseudo-spherical geometry and is valid for nadir observations (for the full range of SCIAMACHY scan angles) up to a solar zenith angle of about 92 degrees. To enable a fast retrieval, a look up table scheme for the radiances and their derivatives has been implemented.

2.1.3 Inversion procedure

WFM-DOAS is a modified DOAS algorithm. A linearised radiative transfer model plus a low order polynomial is linear least squares fitted to the logarithm of the measured sun-normalized radiance. The trace gas vertical profiles are scaled for the fit (i.e., the profile shape is not varied).

Spectral fitting window: 2324.4-2335.0 nm (channel 8)

Fit parameters:

- Scaling factor for CO column
- Scaling factor for methane column
- Scaling factor for H_2O column
- Shift parameter for temperature profile
- Parameters for low order polynomial

In order to minimize systematic biases (due to the channel 8 ice layer, clouds and aerosols, albedo variability, etc.) the CO column is scaled with a dimensionless factor. This factor is the a-priori methane column (computed assuming 3.6E19 molecules/cm^2 for a pixels with a surface elevation at sea level) divided by the simultaneously measured methane column retrieved from the same fitting window.

2.1.4 Averaging kernels

The averaging kernels are available from (ASCII file):
http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/wfmd_averaging_kernels.html

The corresponding a-priori profile is also available from this page (ASCII file). A single profile is used for retrieval (independent of the time and the location of the measurements).

Details concerning the averaging kernels (e.g., how they have been computed) are given in Buchwitz et al., 2004.

2.1.5 Auxiliary data

Atmospheric profiles: US Standard atmosphere with methane and CO_2 scaled to 1750 ppbv and 370 ppmv, respectively. A single profile of temperature, pressure and trace gas mixing ratios is used for all retrievals. These a-priori profiles are available from (ASCII file):
http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/wfmd_averaging_kernels.html

Aerosol scenario: LOWTRAN/MODTRAN aerosol model for tropospheric maritime and normal stratospheric/mesospheric conditions. Details are given in Buchwitz and Burrows, 2004.

Spectroscopic parameters: HITRAN 2004 (the reference is given in Buchwitz et al., 2007a).

2.1.6 Error analysis and algorithm validation

The results of an error analysis of the retrieval with simulated spectra are given in Buchwitz et al., 2004.

Dils et al., 2006b, have performed a comparison for the years 2003 and 2004 with seven European FTIR stations. For 2003 an average bias of +9.2% has been found and a standard deviation of the difference relative to FTIR of +/-20.5%. For 2004 an average bias of +0.5% has been found and a standard deviation of the difference relative to FTIR of +/-21.0%.

The data product has been extensively compared with the CO column data product of MOPITT (see Buchwitz et al., 2007a). Agreement is typically within 20% (with SCIAMACHY typically higher compared to MOPITT especially during 2003 and 2005; for 2004 the average difference SCIAMACHY-MOPITT is close to zero).

2.1.7 Known issues

- No major issues have been identified.

2.1.8 Future work

Analysis of existing years 2003-2005 data set by comparison with independent measurements and model simulations.

Processing and analysis of data after 2005 (depending on funding).

2.2 Methane retrieval algorithm

Algorithm: WFM-DOAS v1.0.

Most relevant reference: Schneising et al., 2009.

Validation: Dils et al., 2006b.

The algorithm is described in detail in Schneising et al., 2009. Here we limit ourselves to a short overview.

2.2.1 Major changes compared to previous version

General information about previous version:

- Algorithm previous version: WFM-DOAS v0.5.
- Most relevant reference: Buchwitz et al., 2006a.
- Validation: Dils et al., 2006a.

Major changes compared to previous version (see also Buchwitz et al., 2006b):

- Use of spectra with improved calibration: Level 1 version 5 (with nominal calibration) instead of (dark signal patched) version 4.
- Use of improved spectroscopy: HITRAN 2004 instead of HITRAN 2000/2001.
- Use of an improved look-up table scheme, e.g., use of an extended set of surface elevations and interpolation of reference spectra with respect to elevation instead of next neighbour approach; three albedos (0.03, 0.1, 0.3) and interpolation scheme instead of only one albedo (0.1).
- Processing of a longer time series: 2003-2005 instead of 2003.
- Optimisation of criteria, which determine a successful measurement (Quality flag).
- The methane data product files now also contain the (XCO_2) CO_2 data product including the O_2 columns retrieved to generate XCO_2. Separate data product files for CH_4 and CO_2 have not been generated any more. Instead the new version 1.0 methane data product files are files for a combined version 1.0 methane and CO_2 data product (this is possible because of the identical methane, CO_2 and O_2 ground pixel size; note that this is not possible for CO because of typically (2x) larger ground pixel size).

2.2.2 Forward model

The forward model is the radiative transfer model SCIATRAN version 1.2 (Buchwitz et al., 2000a). SCIATRAN takes multiple scattering fully into account. SCIATRAN solves the radiative transfer equation for pseudo-spherical geometry and is valid for nadir observations (for the full range of SCIAMACHY scan angles) up to a solar zenith angle of about 92 degrees. To enable a fast retrieval, a look up table scheme for the radiances and their derivatives has been implemented.

2.2.3 Inversion procedure

WFM-DOAS is a modified DOAS algorithm. A linearised radiative transfer model plus a low order polynomial is linear least squares fitted to the logarithm of the measured sun-normalized radiance. The trace gas vertical profiles are scaled for the fit (i.e., the profile shape is not varied).

Spectral fitting window: 1629-1671 nm (channel 6)

Fit parameters:

- Scaling factor for methane column
- Scaling factor for CO_2 column
- Scaling factor for H_2O column
- Shift parameter for temperature profile
- Parameters for low order polynomial

In order to convert the methane column into a mixing ratio (and to minimize systematic biases) the methane column is divided by the dry-air column obtained from the simultaneously retrieved CO_2 column. A constant value of the CO_2 VMR of 370 ppm is assumed. The retrieved CO_2 column is contained in the methane/CO_2 data product.

2.2.4 Averaging kernels

The averaging kernels are available from (ASCII file):
http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/wfmd_averaging_kernels.html

The corresponding a-priori profile is also available from this page (ASCII file). A single profile is used for retrieval (independent of the time and the location of the measurements).

Details concerning the averaging kernels (e.g., how they have been computed) are given in Buchwitz et al., 2005a.

2.2.5 Auxiliary data

Atmospheric profiles: US Standard atmosphere with methane and CO_2 scaled to 1750 ppbv and 370 ppmv, respectively. A single profile of temperature, pressure and trace gas mixing ratios is used for all retrievals. These a-priori profiles are available from (ASCII file):
http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/wfmd_averaging_kernels.html

Aerosol scenario: LOWTRAN/MODTRAN aerosol model for tropospheric maritime and normal stratospheric/mesospheric conditions. Details are given in Buchwitz and Burrows, 2004.

Spectroscopic parameters: HITRAN 2004 (the reference is given in Buchwitz et al., 2007a).

2.2.6 Error analysis and algorithm validation

The results of an error analysis of the retrieval (valid for version 0.4) with simulated spectra are given in Buchwitz et al., 2005a.

The previous version 0.5 data product has been extensively compared with global model simulations (see Buchwitz et al., 2006a). Agreement is typically within a few percent.

Dils et al., 2006b, shows a comparison of the version 1.0 data product for the years 2003 and 2004 with seven European FTIR stations. For 2003 an average bias of –2.7% has been found and a standard deviation of the difference relative to FTIR of +/-1.4%. For 2004 an average bias of -3.5% has been found and a standard deviation of the difference relative to FTIR of +/-1.4%.

2.2.7 Known issues

- No major issues have been identified.

2.2.8 Future work

Analysis of existing years 2003-2005 data set by comparison with independent measurements and model simulations.

Processing and analysis of more data (2006, …).

2.3 Carbon dioxide retrieval algorithm

Algorithm: WFM-DOAS v1.0.

Most relevant references: Buchwitz et al., 2007b, and Schneising et al., 2008.

Validation: Schneising et al., 2008.

The algorithm is described in detail in Schneising et al., 2008. Here we limit ourselves to a short summary.

2.3.1 Major changes compared to previous version

General information about previous version:

- Algorithm previous version: WFM-DOAS v0.4.
- Most relevant reference: Buchwitz et al., 2005a and 2005b; see also Buchwitz et al., 2006a.
- Validation: Dils et al., 2006a.

Major changes compared to previous version (see Schneising et al., 2007a, for details):

- Use of spectra with improved calibration: Level 1 version 5 (with nominal calibration) instead of (dark signal patched) version 4.
- Use of improved spectroscopy: HITRAN 2004 instead of HITRAN 2000/2001.
- Use of an improved look-up table scheme, e.g., use of an extended set of surface elevations and interpolation of reference spectra with respect to elevation instead of next neighbour approach; three albedos (0.03, 0.1, 0.3) and interpolation scheme instead of only one albedo (0.1).
- Processing of a longer time series: 2003-2005 instead of 2003.
- Definition of criteria which determine a successful measurement (Quality flag).
- O_2 fit without albedo weighting function.
- Note: The methane data product files now also contain the (XCO_2) CO_2 data product including the O_2 columns retrieved to generate XCO_2. Separate data product files for CH_4 and CO_2 have not been generated any more. Instead the new version 1.0 methane data product files are files for a combined version 1.0 methane and CO_2 data product (this makes sense because of the identical methane, CO_2 and O_2 ground pixel size; note that this is not possible for CO because of typically larger ground pixel size).

2.3.2 Forward model

The forward model is the radiative transfer model SCIATRAN version 1.2 (Buchwitz et al., 2000a). SCIATRAN takes multiple scattering fully into account. SCIATRAN solves the radiative transfer equation for pseudo-spherical geometry and is valid for nadir observations (for the full range of SCIAMACHY scan angles) up to a solar zenith angle of about 92 degrees. To enable a fast retrieval, a look up table scheme for the radiances and their derivatives has been implemented.

2.3.3 Inversion procedure

WFM-DOAS is a modified DOAS algorithm. A linearised radiative transfer model plus a low order polynomial is linear least squares fitted to the logarithm of the measured sun-normalized radiance. The trace gas vertical profiles are scaled for the fit (i.e., the profile shape is not varied).

Spectral fitting window: 1558-1594 nm (channel 6)

Fit parameters:

- Scaling factor for CO_2 column
- Scaling factor for H_2O column
- Shift parameter for temperature profile
- Parameters for low order polynomial

In order to convert the CO_2 column into a mixing ratio the CO_2 column is divided by the dry-air column obtained from the simultaneously measured O_2 column obtained from the O_2 A band.

Details O_2 fit:

Spectral fitting window: 755-775 nm (channel 4)

Fit parameters:

- Scaling factor for O_2 column
- Shift parameter for temperature profile
- Parameters for low order polynomial

2.3.4 Averaging kernels

The averaging kernels are available from (ASCII file):
http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/wfmd_averaging_kernels.html

The corresponding a-priori profile is also available from this page (ASCII file). A single profile is used for retrieval (independent of the time and the location of the measurements).

Details concerning the averaging kernels (e.g., how they have been computed) are given in Buchwitz et al., 2005a.

2.3.5 Auxiliary data

Atmospheric profiles: US Standard atmosphere with methane and CO_2 scaled to 1750 ppb and 370 ppm, respectively. A single profile of temperature, pressure and trace gas mixing ratios is used for all retrievals. These a-priori profiles are available from (ASCII file):
http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/wfmd_averaging_kernels.html

Aerosol scenario: LOWTRAN/MODTRAN aerosol model for tropospheric maritime and normal stratospheric/mesospheric conditions. Details are given in Buchwitz and Burrows, 2004.

Spectroscopic parameters: HITRAN 2004 (the reference is given in Buchwitz et al., 2007a).

2.3.6 Error analysis and algorithm validation

The results of an error analysis of the retrieval with simulated spectra is given in Schneising et al., 2008.

Validation by comparison with independent measurements:

- For the previous version 0.4 product see Dils et al., 2006a.
- For the current version 1.0 see Schneising et al., 2008 (see also Buchwitz et al., 2007b). Based on a comparison with a (very) limited number of ground-based FTS measurements and global model simulations our current error estimates are: Single pixel retrieval precision: 2-3% (~9 ppm). Systematic low bias of ~1.5%. Relative accuracy ~1-2% for monthly XCO2 over land at 7 deg x 7 deg horizontal resolution.

2.3.7 Known issues

- No major problems have been identified

2.3.8 Future work

Analysis of existing years 2003-2005 data set by comparison with independent measurements and model simulations.

Processing and analysis of more data (2006, …).

3 Product specification

3.1 General

To satisfy the needs of most of the WFM-DOAS data products user three different types or levels of data products have been generated:

Level 2a:

This is the basic data product (lowest level), which contains "all" processed data (not only the data classified "good").

One (ASCII) file (*.was) is provided per orbit (for CO; for XCH4 and XCO2 an additional auxiliary file (*.wasaux) is provided for each orbit containing important additional information, e.g., the "final" XCH4 and XCO2 quality flags).

Each file contains a header followed by a table of data. The header contains a description of the columns of the table of data. The table contains for each ground pixel the main product, its estimated error, and a quality flag to indicate if the measurement is "good" plus a large number of auxiliary information such as measurement time, geolocation information (latitude and longitude), solar zenith angle, etc. Each row of the table corresponds to a single ground pixel (scene).

File name extension: was (= WFM-DOAS ASCII file).

This data product is for users who are interested not only in data classified "good" (as defined by the quality flag) but, for example, want to investigate CO_2 over water or retrieval results for significantly cloud contaminated scenes.

Level 2b:

This data product is a sub-set of the Level 2a product. One file is provided for each month containing only the data classified as "good" (as defined by the quality flag). The structure of these files is similar as for Level 2a.

File name extension: was (= WFM-DOAS ASCII file).

This data product is for users who are only interested in data which are classified "good" and need detailed ground pixel time/geolocation information.

Level 3:

This data product contains the gridded data (0.5 deg latitude x 0.5 deg longitude) at monthly resolution. Each (ASCII) file contains a header followed by a matrix of data. Four data files have been generated for each month:

- Main data product, i.e., the CO column or the greenhouse gas column-averaged mole fraction
- The mean fit error (in percent)
- The standard deviation of the measurements that have been averaged for a given grid cell (in percent)
- The number of measurements per grid cell

File name extension: grid.

This data product is for users who are only interested in data, which are classified “good” and are happy with monthly time resolution.

3.2 Carbon monoxide product specification

3.2.1 Processed data

All available data of the years 2003-2005.

3.2.2 Validation

The data product has been extensively compared with the CO column data product of MOPITT (see Buchwitz et al., 2007a). Agreement is typically within 20% (with SCIAMACHY typically somewhat higher compared to MOPITT especially during 2003 and 2005).

Dils et al., 2006b, shows a comparison for the years 2003 and 2004 with seven European FTIR stations. For 2003 an average bias of +9.2% has been found and a standard deviation of the difference relative to FTIR of +/-20.5%. For 2004 an average bias of +0.5% has been found and a standard deviation of the difference relative to FTIR of +/-21.0%.

3.2.3 Known issues related to the product files

- No issues have been identified

3.2.4 Product description: CO Level2a_orbits_swath_QUALall

The SCIAMACHY WFM-DOAS product files are ASCII files consisting of a detailed header followed by a table with the data (one line per ground pixel). For each orbit one product file is generated. The horizontal resolution is typically: 30 x 120 km^2.

An example of the file header is given on the following page. This file header contains a description of the content of all columns of the table of data that follows after the header.

Here we provide additional information for those columns where we think that additional information is needed:

Column#	**Comments**
3	Pixel type: 1 = nominal forward scan ground pixel; 2 = fast backscan pixel
19	Cloud mask: 0 = cloud free; 1 = cloud contaminated
20	Land mask: 0 = full pixel or part of pixel over water; 1 = land pixel
22	Absolute value of SCIAMACHY measured sun-normalized radiance
Main CO product:	
30	CO product in molecules/cm2
31	Percentage error of CO product. Computed taking into account the quality of the spectral fit (RMS of fit residuum). The explicit formula is given in Buchwitz et al., 2004.
32	CO product quality flag 0 = quality OK 1 = quality not OK The quality flag is determined using a number of criteria: Quality OK if: RMS of fit residuum < 0.02; CO fiterror less than 1.2E18 molec/cm^2 and less than 100%; CO column positive and less than 1e19 molec/cm^2; CH4 columns within 30% of assumed (a-priori) column (= 3.6E19 molec/cm^2 for a ground pixel with an average surface elevation corresponding to sea level); SZA less than 88 deg; forward scan pixel (i.e., no fast back scan pixel because of four times larger ground pixel size). Note: The quality flag is independent of the land mask and of the cloud mask.

Example of CO Level 2a product file header:

```
# CO total columns from SCIAMACHY/ENVISAT orbit 08663_3726.SCIA_2003 day 20031027
# Generated by Michael.Buchwitz@iup.physik.uni-bremen.de on Tue Jul 18 06:49:25 …
# Level 1b file:    SCI_NL__1PPDPA20031027_063414_000060482021_00092_08663_3726.N1
# Sensing start:    27-OCT-2003 06:34:14.360974
# Sensing stop :    27-OCT-2003 08:15:02.497401
# Channel:   8
# Fitwindow: 2324.4 2335.0 nm
# Col 0: px#        : Ground pixel number (per orbit) [-] (1,2,...)
# Col 1: st#        : State number [-] (0,1,..)
# Col 2: read#      : Ground pixel number (per state) [-] (0,1,...)
# Col 3: t          : Pixel type [-] (1:forward 2:backscan)
# Col 4: dsr_time   : Starttime in frac.days since 1.1.2000 [day]
# Col 5: t_int      : Integration time [s]
# Col 6: lat_c      : Latitude  center   [deg]
# Col 7: lon_c      : Longitude center   [deg]
# Col 8: lat_1      : Latitude  corner 1 [deg]
# Col 9: lon_1      : Longitude corner 1 [deg]
# Col10: lat_2      : Latitude  corner 2 [deg]
# Col11: lon_2      : Longitude corner 2 [deg]
# Col12: lat_3      : Latitude  corner 3 [deg]
# Col13: lon_3      : Longitude corner 3 [deg]
# Col14: lat_4      : Latitude  corner 4 [deg]
# Col15: lon_4      : Longitude corner 4 [deg]
# Col16: sza        : Solar zenith angle [deg]
# Col17: los        : Line-of-sight zenith angle [deg]
# Col18: azi        : Relative azimuth angle [deg]
# Col19: cld        : Cloud mask (1: probably cloud contamin.)
# Col20: lnd        : Land mask (1: completely land covered)
# Col21: rms        : RMS of fit residuum [-]
# Col22: snrad      : Sun-normalized radiance (no data=-0.99999D+00)
# Col23: alt        : Average ground altitude [km]
# Col24: H2O        : H2O column [molec./cm2]
# Col25: H2O_err    : H2O column error [%]
# Col26: CH4        : CH4 column [molec./cm2]
# Col27: CH4_err    : CH4 column error [%]
# Col28: CO         : CO column [molec./cm2]
# Col29: CO_err     : CO column error [%]
# Col30: CO_corr    : CO product [molec./cm2]
# Col31: CO_corr_err: CO product error [%]
# Col32: CO_qual    : CO product quality flag (1: bad)
#  px# st# read# t      dsr_time    t_int   lat_c     lon_c     lat_1     lon_1  …
```

…

Table with data

…

3.2.5 Product description: CO Level2b_orbits_swath_QUALgood

This data product is a sub-set of the Level 2a product. One file is provided for each month containing only the “good” data (as defined by the quality flag). The structure of these files is similar as for Level 2a.

An example file header is given on the next page.

The final CO product is contained in columns 30-32:

```
# Col30: CO_corr     : FINAL CO product [molec./cm2]
# Col31: CO_corr_err: FINAL CO product error [%]
# Col32: CO_qual     : FINAL CO product quality flag (1: bad, 0: good)
```

Example of CO Level 2b product file header:

```
# CO total columns from SCIAMACHY/ENVISAT WFM-DOAS version 0.6 Year 2003 Month 10
# Generated by Michael.Buchwitz@iup.physik.uni-bremen.de
# Contains only measurements with QUALITY = OK
# Channel:   8
# Fitwindow: 2324.4 2335.0 nm
# Col 0: px#         : Ground pixel number (per orbit) [-] (1,2,...)
# Col 1: st#         : State number [-] (0,1,..)
# Col 2: read#       : Ground pixel number (per state) [-] (0,1,...)
# Col 3: t           : Pixel type [-] (1:forward 2:backscan)
# Col 4: dsr_time    : Starttime in frac.days since 1.1.2000 [day] (0 = 1 Jan 2000)
# Col 5: t_int       : Integration time [s]
# Col 6: lat_c       : Latitude  center   [deg]
# Col 7: lon_c       : Longitude center   [deg]
# Col 8: lat_1       : Latitude  corner 1 [deg]
# Col 9: lon_1       : Longitude corner 1 [deg]
# Col10: lat_2       : Latitude  corner 2 [deg]
# Col11: lon_2       : Longitude corner 2 [deg]
# Col12: lat_3       : Latitude  corner 3 [deg]
# Col13: lon_3       : Longitude corner 3 [deg]
# Col14: lat_4       : Latitude  corner 4 [deg]
# Col15: lon_4       : Longitude corner 4 [deg]
# Col16: sza         : Solar zenith angle [deg]
# Col17: los         : Line-of-sight zenith angle [deg]
# Col18: azi         : Relative azimuth angle [deg]
# Col19: cld         : Cloud mask (1: cloud contaminated, 0: cloud free)
# Col20: lnd         : Land mask (1: completely land covered)
# Col21: rms         : RMS of fit residuum [-]
# Col22: snrad       : Sun-normalized radiance (no data=-0.99999D+00)
# Col23: alt         : Average ground altitude [km]
# Col24: H2O         : H2O column [molec./cm2]
# Col25: H2O_err     : H2O column error [%]
# Col26: CH4         : CH4 column [molec./cm2]
# Col27: CH4_err     : CH4 column error [%]
# Col28: CO          : CO column [molec./cm2]
# Col29: CO_err      : CO column error [%]
# Col30: CO_corr     : FINAL CO product [molec./cm2]
# Col31: CO_corr_err: FINAL CO product error [%]
# Col32: CO_qual     : FINAL CO product quality flag (1: bad, 0: good)
#  px# st# read# t      dsr_time    t_int   lat_c     lon_c     lat_1     …
```

…

Table with data

…

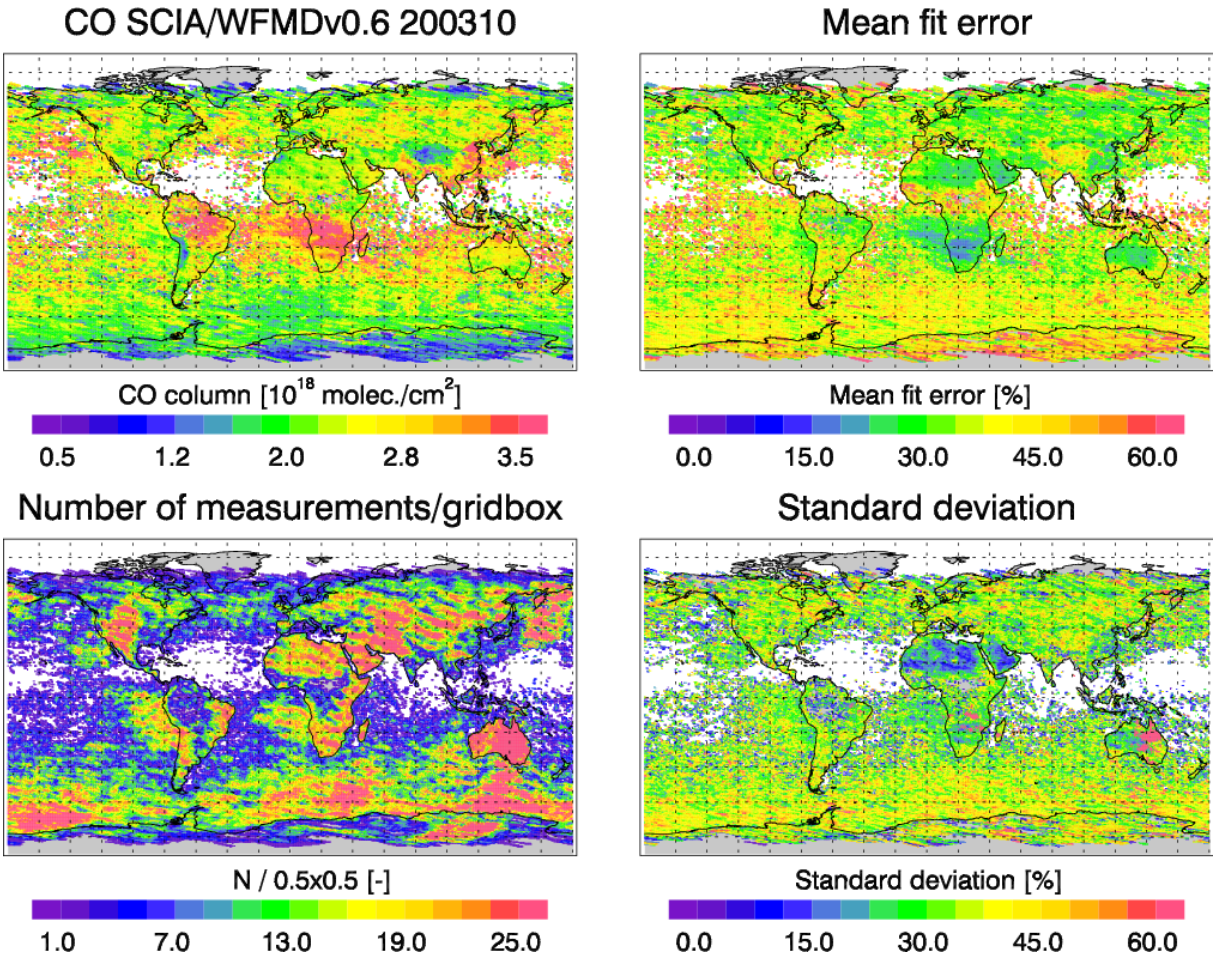
3.2.6 Product description: CO Level3_monthly_grid_QUALgood

This data product contains the gridded data (0.5 deg latitude x 0.5 deg longitude) at monthly resolution produced from the corresponding Level 2b file.

Each (ASCII) file contains a header followed by a matrix of data. Four data files have been generated for each month:

- Main data product, i.e., the CO column
- The mean fit error (in percent)
- The standard deviation of the measurements that have been averaged for a given grid cell (in percent)
- The number of measurements per grid cell

The file name extension is “grid”. Here the content of the grid files for October 2003:



Description of the grid files:

General:

Spatial resolution: 0.5 deg latitude x 0.5 deg longitude.
Temporal resolution: monthly.

File name extension: grid (*.grid)

File structure:
ASCII. Two header lines starting with "#"
followed by a table (matrix) containing the data (see below).

Main directory:

`./Level3_monthly_grid_QUALgood/`

Sub-directories:

`./columns/*col*.grid`
SCIAMACHY WFM-DOAS version 0.6 CO columns in molecules/cm^2.

`./fiterror/*err*.grid`
Mean CO fit error in percent.

`./stddev/*std*.grid`
Standard deviation in percent.

`./npts_per_gridbox*n__*.grid`
Number of measurements per grid cell.

`./lat_lon/*.grid`
Latitude and longitude grid-files.

`./figures_png/*.png`
One plot for each month showing each of the four grid files (column, fiterror, stddev, number of points).

Description of the data matrix:

Dimension: NumberOfLongitudes x NumberOfLongitudes
NumberOfLongitudes = 720 ; NumberOfLatitudes = 360

Which longitudes and latitudes?
The centre latitudes and longitudes for each grid cell are given in the `./lat_lon/longitudes.grid` and `./lat_lon/latitudes.grid` grid files.

These files have the same structure as (all) the other (main product) grid files, i.e., each file contains a matrix which has the same structure as the matrix contained in the other (main product) grid files.

The range of longitude values is: 0 deg to 360 deg
The first 5 (grid cell centre) longitudes are:
`2.5000e-01  7.5000e-01  1.2500e+00  1.7500e+00  2.2500e+00 …`

The range of latitude values is: -90 deg to 90 deg
The first 5 (grid cell centre) latitudes are (all identical):
`-8.9750e+01 -8.9750e+01 -8.9750e+01 -8.9750e+01 -8.9750e+01 …`

Here an example how to read the grid files using IDL:

```
co_file       ='./columns/SCIA_CO_col_WFMDv06_200301.grid'
;             CO columns for January 2003 (=200301)
latitude_file ='./lat_lon/latitudes.grid'
longitude_file='./lat_lon/longitudes.grid'
nlon=720 ; number of longitudes
nlat=360 ; number of latitudes
;
str='string'
co=fltarr(nlon,nlat)
openr,1, co_file
readf, 1, str
readf, 1, str
readf, 1, co
close, 1
lat=fltarr(nlon,nlat)
openr,1, latitude_file
readf, 1, str
readf, 1, str
readf, 1, lat      ; gridcell center latitude in degrees from -90.0 to +90.0
close, 1
lon=fltarr(nlon,nlat)
openr,1, longitude_file
readf, 1, str
readf, 1, str
readf, 1, lon     ; gridcell center longitude in degrees from 0 to 360
close, 1
;
; Now matrix co contains the CO columns.
; The rectangular lat/lon region corresponding to co(i,j) is:
; Latitude range : From lat(i,j)-0.25 to lat(i,j)+0.25
; Longitude range: From lon(i,j)-0.25 to lon(i,j)+0.25
```

3.3 Methane product specification

3.3.1 Processed data

All available data of the years 2003-2005.

3.3.2 Validation

Dils et al., 2006b, shows a comparison of the version 1.0 data product for the years 2003 and 2004 with seven European FTIR stations. For 2003 an average bias of –2.7% has been found and a standard deviation of the difference relative to FTIR of +/-1.4%. For 2004 an average bias of -3.5% has been found and a standard deviation of the difference relative to FTIR of +/-1.4%.

In Schneising et al., 2009, detailed comparisons with global model data (TM5 model) for 2003 are given. It has been found that after accounting for a low bias of ~2% (for the not CO_2 corrected XCH_4; for the CO_2 corrected XCH_4 the bias is ~1%) agreement with TM5 is typically within 1-2%.

3.3.3 Known issues related to the product files

- No major issues have been identified.

3.3.4 Product description: XCH4 Level2a_orbits_swath_QUALall

The SCIAMACHY WFM-DOAS Level 2a product files are ASCII files consisting of a header followed by a table with data (one line per ground pixel). The header contains a detailed description of the contents of the columns of the table (an example header is given below).

Please note that the Level 2 XCH4 and XCO2 products are provided in the SAME file, which contains BOTH products.

The horizontal resolution is typically 30 x 60 km^2 (for both XCH4 and XCO2).

For each orbit TWO product files are generated (for historical reasons):

The main Level 2a orbit "**was**" file (*.was) and an additional file with important additional auxiliary information (*.wasaux) which has an identical filename as the was file but a different extension, namely "**wasaux**".

The number of header lines of the was files and the corresponding wasaux files are identical.

The number of data lines of a was file and its corresponding wasaux file are identical. This is because the wasaux file simply provides additional columns for the table contained in the was file and therefore must have the same number of rows. Each (non-header) line in a was file corresponds to a (non-header) line in the corresponding wasaux file at the same line number, i.e., line 1111 in the was file and line 1111 in the corresponding wasaux file refer to the SAME ground pixel.

Please note that the wasaux file is needed because it contains the final XCH4 and XCO2 quality flags:

```
# Col16: XCO2FQ      : XCO2 final quality flag (0:good 1:bad)
...
# Col19: XCH4FQ      : XCH4 final quality flag (0:good 1:bad)
```

For the convenience of the user we have copied the most relevant information from the was file into the wasaux file (time, geolocation, XCH4, XCO2, their errors, etc). **Therefore, for most applications, only the wasaux file is needed.**

An example of the Level 2a was file header is given on the following page. This file header contains a description of the content of all columns of the table of data that follows after the header.

Here we provide additional information for those columns where we think that additional information is needed:

Column#	**Comments**
3	Pixel type: 1 = nominal forward scan ground pixel; 2 = fast backscan pixel
19	Cloud mask: 0 = cloud free; 1 = cloud contaminated
20	Land mask: 0 = full pixel or part of pixel over water; 1 = land pixel
21	Absolute value of SCIAMACHY measured sun-normalized radiance
Main methane product:	
44	XCH4 product in ppbv
45	Percentage error of XCH4 product. Computed taking into account the quality of the spectral fit (RMS of fit residuum). The explicit formula is given in Buchwitz et al., 2005a.
46	XCH4 product quality flag 0 = quality OK 1 = quality not OK The XCH4 quality flag is determined using a number of criteria. Quality OK if: CH4 RMS fit residuum < 0.004; CO2 RMS fit residuum < 0.0025; O2 RMS fit residuum < 0.025; CH4 column fit errors less than 4%; O2 column larger than 90% of assumed (a-priori) column (= 4.5E24molecules/cm2 for a ground pixel with an average surface elevation corresponding to sea level); SZA less than 75 deg. <u>Important notes:</u> In addition to the XCH4 quality flag we recommend to use the following filter criteria (in addition!): XCO2 quality flag = 0 (column 39) Pixel type = 1 (forward scan; column 3) Note: The XCH4 and XCO2 quality flags are independent of the land mask and of the cloud mask. **Note: It is strongly recommended to use the optimised final quality flag provided in the corresponding wasaux file !**

Example of methane (and CO_2) Level 2a product file header (was file):

```
# CO2 and CH4 total columns from SCIAMACHY/ENVISAT orbit 08663_3726.SCIA_2003 …
# Generated by Oliver.Schneising@iup.physik.uni-bremen.de on Fr Sep 22 …
# Level 1b file:    SCI_NL__1PPDPA20031027_063414_000060482021_00092_08663_3726.N1
# Sensing start:    27-OCT-2003 06:34:14.360974
# Sensing stop :    27-OCT-2003 08:15:02.497401
# Channel      :        6
# Fitwindows   :        1558.0 1594.0 nm (CO2) / 1630.0 1671.0 nm (CH4)
# Col 0: px#         : Ground pixel number (per orbit) [-] (1,2,...)
# Col 1: st#         : State number [-] (0,1,..)
# Col 2: read#       : Ground pixel number (per state) [-] (0,1,...)
# Col 3: t           : Pixel type [-] (1:forward 2:backscan)
# Col 4: dsr_time    : Starttime in frac.days since 1.1.2000 [day]
# Col 5: t_int       : Integration time [s]
# Col 6: lat_c       : Latitude  center   [deg]
# Col 7: lon_c       : Longitude center   [deg]
# Col 8: lat_1       : Latitude  corner 1 [deg]
# Col 9: lon_1       : Longitude corner 1 [deg]
# Col10: lat_2       : Latitude  corner 2 [deg]
# Col11: lon_2       : Longitude corner 2 [deg]
# Col12: lat_3       : Latitude  corner 3 [deg]
# Col13: lon_3       : Longitude corner 3 [deg]
# Col14: lat_4       : Latitude  corner 4 [deg]
# Col15: lon_4       : Longitude corner 4 [deg]
# Col16: sza         : Solar zenith angle [deg]
# Col17: los         : Line-of-sight zenith angle [deg]
# Col18: azi         : Relative azimuth angle [deg]
# Col19: cld         : Cloud mask (1: probably cloud contamin.)
# Col20: lnd         : Land mask (1: completely land covered)
# Col21: snrad       : Sun-normalized radiance (R/I*PI) [-]
# Col22: alt         : Average ground altitude [km]
# Col23: H2O(CH4 fit): H2O column of CH4 fit [molec./cm2]
# Col24: H2O_err(CH4): H2O column error of CH4 fit [%]
# Col25: H2O(CO2 fit): H2O column of CO2 fit [molec./cm2]
# Col26: H2O_err(CO2): H2O column error of CO2 fit [%]
# Col27: O2#         : Number of O2 (sub-)pixel [-]
# Col28: O2          : O2 column [molec./cm2]
# Col29: O2_err      : O2 column error [%]
# Col30: O2_rms      : RMS of O2 fit residuum [-]
# Col31: O2_qual     : O2 quality flag (1: bad)
# Col32: CO2#        : Number of CO2 (sub-)pixel [-]
# Col33: CO2         : CO2 column [molec./cm2]
# Col34: CO2_err     : CO2 column error [%]
# Col35: CO2_rms     : RMS of CO2 fit residuum [-]
# Col36: CO2_qual    : CO2 quality flag (1: bad)
# Col37: XCO2        : XCO2 [ppmv]
# Col38: XCO2_err    : XCO2 error [%]
# Col39: XCO2_qual   : XCO2 quality flag (1: bad)
# Col40: CH4         : CH4 column [molec./cm2]
# Col41: CH4_err     : CH4 column error [%]
# Col42: CH4_rms     : RMS of CH4 fit residuum [-]
# Col43: CH4_qual    : CH4 quality flag (1: bad)
# Col44: XCH4        : XCH4 [ppbv]
# Col45: XCH4_err    : XCH4 error [%]
# Col46: XCH4_qual   : XCH4 quality flag (1: bad)
#  px# st# read# t      dsr_time    t_int   lat_c     lon_c     lat_1 ...
```

…

Table with data

…

Header of corresponding Level2a wasaux file:

```
# CO2 and CH4 mole fractions from SCIAMACHY/ENVISAT orbit 08663_3726 day 20031027
# Generated by Oliver.Schneising@iup.physik.uni-bremen.de on Fr Mai 25 05:10:00 …
# Retrieval algorithm: WFM-DOAS version 1.0
#
# Channel    : 6
# Fitwindows : 1558.0 1594.0 nm (CO2) / 1630.0 1671.0 nm (CH4)
#
#
# Col 0: px#          : Ground pixel number (per orbit) [-] (1,2,...)
# Col 1: dsr_time     : Starttime in fractional days since 1.1.2000 [day] (0.x=1….
# Col 2: lat_c        : Latitude  center   [deg]
# Col 3: lon_c        : Longitude center   [deg]
# Col 4: lat_1        : Latitude  corner 1 [deg]
# Col 5: lon_1        : Longitude corner 1 [deg]
# Col 6: lat_2        : Latitude  corner 2 [deg]
# Col 7: lon_2        : Longitude corner 2 [deg]
# Col 8: lat_3        : Latitude  corner 3 [deg]
# Col 9: lon_3        : Longitude corner 3 [deg]
# Col10: lat_4        : Latitude  corner 4 [deg]
# Col11: lon_4        : Longitude corner 4 [deg]
# Col12: o2_apri      : O2 a-priori column [molec./cm2]
# Col13: aer          : Aerosol mask (0:normal/OK 1:aerosol contaminated 2:…
# Col14: XCO2         : XCO2 [ppm]
# Col15: XCO2_err     : XCO2 error [%]
# Col16: XCO2FQ       : XCO2 final quality flag (0:good 1:bad)
# Col17: XCH4         : XCH4 [ppb]
# Col18: XCH4_err     : XCH4 error [%]
# Col19: XCH4FQ       : XCH4 final quality flag (0:good 1:bad)
#
#
#
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#
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#
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#
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#
#
#
#
#
#
#
#
#
#
#
#
#
#  px#       dsr_time   lat_c     lon_c     lat_1     lon_1     lat_2  …
```

3.3.5 Product description: XCH4 Level2b_monthly_swath_QUALgood

This data product is a sub-set of the Level 2a product. One file is provided for each month containing only the “good” Level 2a data (as defined by the quality flag). The structure of these files is similar as for Level 2a.

An example file header is given on the following page.

The final XCH4 product is contained in the following columns:

```
# Col44: XCH4          : XCH4 [ppb]
# Col45: XCH4_err      : XCH4 error [%]
...
# Col48: XCH4FQ        : XCH4 final quality flag (0:good 1:bad)
```

Column 48 which contains the final XCH4 quality flag comes from / is identical with the final quality flag contained in the Level 2a wasaux file.

Example of XCH4 (=XCO2) Level 2b product file header:

```
# CO2 and CH4 total columns and mole fractions from SCIAMACHY/ENVISAT Month 200310
# Generated by Oliver.Schneising@iup.physik.uni-bremen.de on Do Mai 31 …
# Retrieval algorithm : WFM-DOAS version 1.0
# Channel             : 6
# Fitwindows          : 1558.0 1594.0 nm (CO2) / 1630.0 1671.0 nm (CH4)
# Col 0: px#          : Ground pixel number (per orbit) [-] (1,2,...)
# Col 1: st#          : State number [-] (0,1,..)
# Col 2: read#        : Ground pixel number (per state) [-] (0,1,...)
# Col 3: t            : Pixel type [-] (1:forward 2:backscan)
# Col 4: dsr_time     : Starttime in fractional days since 1.1.2000 [day] (0.x = …
# Col 5: t_int        : Integration time [s]
# Col 6: lat_c        : Latitude  center   [deg]
# Col 7: lon_c        : Longitude center   [deg]
# Col 8: lat_1        : Latitude  corner 1 [deg]
# Col 9: lon_1        : Longitude corner 1 [deg]
# Col10: lat_2        : Latitude  corner 2 [deg]
# Col11: lon_2        : Longitude corner 2 [deg]
# Col12: lat_3        : Latitude  corner 3 [deg]
# Col13: lon_3        : Longitude corner 3 [deg]
# Col14: lat_4        : Latitude  corner 4 [deg]
# Col15: lon_4        : Longitude corner 4 [deg]
# Col16: sza          : Solar zenith angle [deg]
# Col17: los          : Line-of-sight zenith angle [deg]
# Col18: azi          : Relative azimuth angle [deg]
# Col19: cld          : PMD cloud mask (1:probably cloud contaminated)
# Col20: lnd          : Land mask (1:completely land covered)
# Col21: snrad        : Sun-normalized radiance (R/I*PI) [-]
# Col22: alt          : Average ground altitude [km]
# Col23: H2O(CH4 fit) : H2O column of CH4 fit [molec./cm2]
# Col24: H2O_err(CH4) : H2O column error of CH4 fit [%]
# Col25: H2O(CO2 fit) : H2O column of CO2 fit [molec./cm2]
# Col26: H2O_err(CO2) : H2O column error of CO2 fit [%]
# Col27: O2#          : Number of O2 (sub-)pixel [-]
# Col28: O2           : O2 column [molec./cm2]
# Col29: O2_err       : O2 column error [%]
# Col30: O2_rms       : RMS of O2 fit residuum [-]
# Col31: O2Q          : O2 quality flag (0:good 1:bad)
# Col32: CO2#         : Number of CO2 (sub-)pixel [-]
# Col33: CO2          : CO2 column [molec./cm2]
# Col34: CO2_err      : CO2 column error [%]
# Col35: CO2_rms      : RMS of CO2 fit residuum [-]
# Col36: CO2Q         : CO2 quality flag (0:good 1:bad)
# Col37: XCO2         : XCO2 [ppm]
# Col38: XCO2_err     : XCO2 error [%]
# Col39: XCO2Q        : XCO2 quality flag (0:good 1:bad)
# Col40: CH4          : CH4 column [molec./cm2]
# Col41: CH4_err      : CH4 column error [%]
# Col42: CH4_rms      : RMS of CH4 fit residuum [-]
# Col43: CH4Q         : CH4 quality flag (0:good 1:bad)
# Col44: XCH4         : XCH4 [ppb]
# Col45: XCH4_err     : XCH4 error [%]
# Col46: XCH4Q        : XCH4 quality flag (0:good 1:bad)
# Col47: XCO2FQ       : XCO2 final quality flag (0:good 1:bad)
# Col48: XCH4FQ       : XCH4 final quality flag (0:good 1:bad)
#  px# st# read# t      dsr_time    t_int   lat_c     lon_c     lat_1 …
```

3.3.6 Product description: XCH4 Level3_monthly_grid_QUALgood

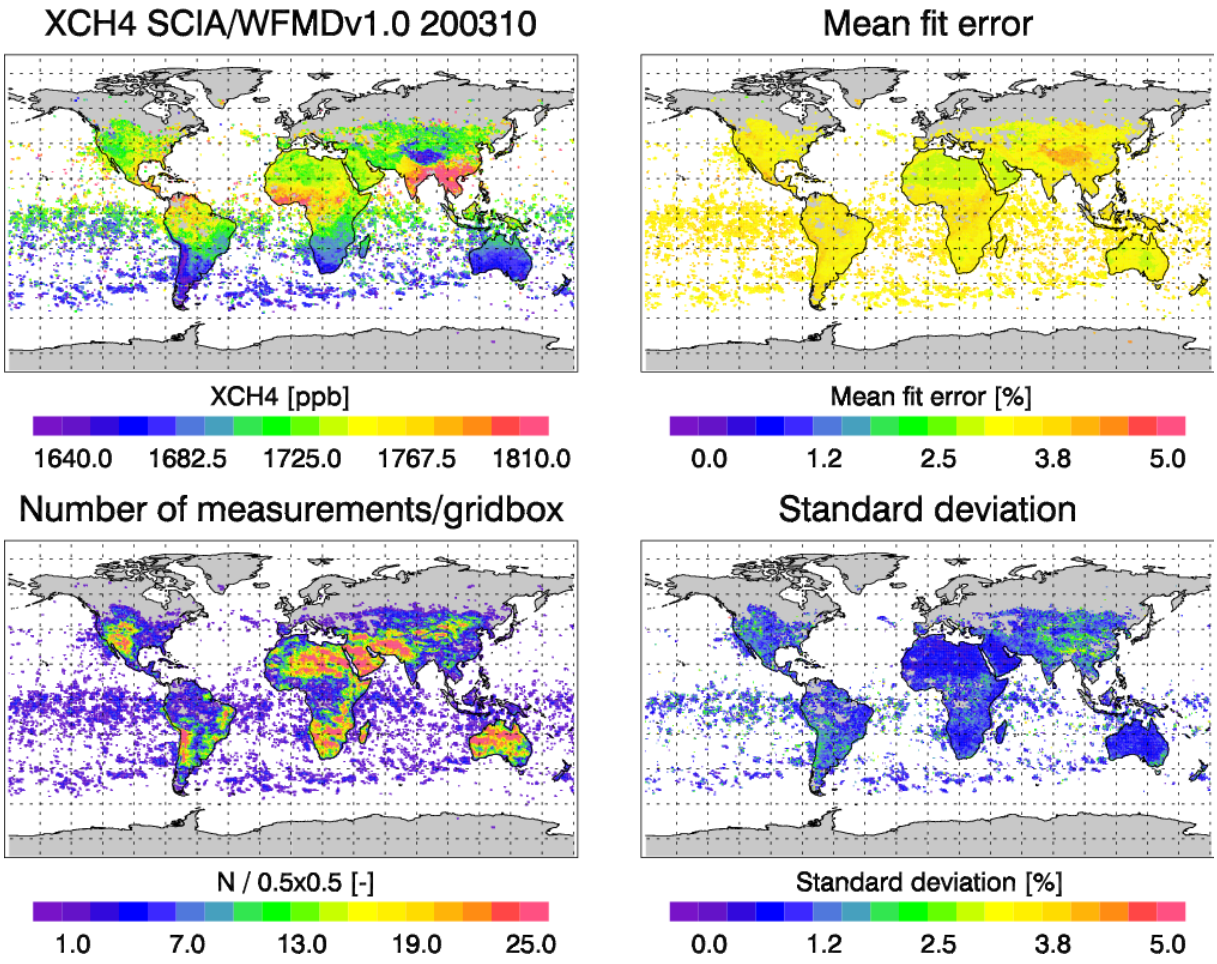
This data product contains the gridded data (0.5 deg latitude x 0.5 deg longitude) at monthly resolution produced from the corresponding Level 2b file.

Each (ASCII) file contains a header followed by a matrix of data.

The file name extension is “grid”.

The structure of the XCH4 grid files is identical with the structure of the CO column data product grid file described in **Section 3.2.6**.

Here the content of the grid files for October 2003:



3.3.7 Product description: XCH4: Important final remarks

As described in Schneising et al., 2009, the accuracy of the SCIAMACHY XCH4 product can be improved by using a CO_2 correction (using NOAA's CarbonTracker).

This CO_2 corrected methane data product can now also be downloaded from the University of Bremen SCIAMACHY/WFM-DOAS web site. The CO2 corrected methane data products are stored in directories (and filenames) containing the contain substring "ccs" (= "CO_2 corrected & scaled"):

- **Level 3** (CO_2 corrected CH4 v1.0 product, scaled with x1.01 to correct for 1% low bias as described in Schneising et al., 2009): Directory **Level3_XCH4ccs_monthly_grid_QUALgood/** has the same structure as directory Level3_XCH4_monthly_grid_QUALgood/, which contains the original (not CO_2 corrected, not scaled) product.
- **Level 2b:** Directory **Level2b_XCH4ccs_monthly_swath_QUALgood/** contains file **SCIA_XCH4v1_wasaux2.tar.gz**, which contains *.wasaux2 files (one per month). Each line (row) of a *.wasaux2 file corresponds exactly to one line (same row) of the "full" Level 2b file, i.e. *.was file located in directory Level2b_monthly_swath_QUALgood/ This meas that for each *.was file (containing time info, geolocation info etc) a corresponding *.wasaus2 file exists containing the CO_2 corrected and scaled XCH_4.

Although the spatial pattern are only moderately affected (see Schneising et al., 2009**) it is highly recommended to use the CO_2-corrected XCH_4 product instead of the not corrected one** because of higher accuracy!

3.4 Carbon dioxide product specification

3.4.1 Processed data

All available data of the years 2003-2005.

3.4.2 Validation

Details are given in Schneising et al., 2008. Based on a comparison with a very limited number of ground-based FTS measurements and global model simulations our current error estimates are:
Single pixel retrieval precision: ~2% (~8 ppm).
Systematic low bias of ~1.5%.
Relative accuracy ~1-2% for monthly XCO_2 over land at 7 deg x 7 deg horizontal resolution.

3.4.3 Known issues related to the product files

- No major issues have been identified.

3.4.4 Product description: XCO2 Level2a_orbits_swath_QUALall

The Level 2a XCO2 and XCH4 products are provided in the SAME file which contains BOTH products.

A file format description is given in **Section 3.3.4** where the Level 2a XCH4 product is described.

Please note that all remarks given in Section 3.3.4 related to the *.was and *.wasaux files are also relevant for XCO2.

Here we give some additional information related to the CO_2 product:

Column#	**Comments**
Main XCO2 product:	
37	XCO2 product in ppmv
38	Percentage error of XCO2 product. Computed taking into account the quality of the spectral fit (RMS of fit residuum). The explicit formula is given in Buchwitz et al., 2005a.
39	XCO2 product quality flag 0 = quality OK 1 = quality not OK The XCO2 quality flag is determined using a number of criteria. Quality OK if: CO2 RMS fit residuum < 0.0025; O2 RMS fit residuum < 0.02; CO2 column fit error less than 2.5%; O2 column larger than 90% of assumed (a-priori) column (= 4.5E24 molecules/cm2 for a ground pixel with an average surface elevation corresponding to sea level); SZA less than 75 deg. <u>Important notes:</u> In addition to the XCO2 quality flag we recommend to use also the following filter criteria: Pixel type = 1 (forward scan; column 3); Cloud mask = 0 (cloud free; column 19); Land mask = 1 (land pixel; column 20) **Note: It is strongly recommended to use the optimised final quality flag provided in the corresponding wasaux file !** In addition to the refined quality criteria given above the final quality flag as given in the wasaux file also takes into account strong aerosol contamination as identified using NASA's TOMS/Earthprobe Absorbing Aerosol Index (AAI). For details see Schneising et al., 2007a.

Examples of Level 2a XCO2 was and wasaux product file header: See XCH4 product file headers in **Section 3.3.4.**

3.4.5 Product description: XCO2 Level2b_monthly_swath_QUALgood

The XCO2 Level 2b product file is identical with the XCH4 Level 2b product file (both products are contained in the same files because of identical spatial resolution).

As for XCH4, this data product is a sub-set of the Level 2a product.

One file is provided for each month containing only the “good” data (as defined by the quality flag).

The structure of these files is similar as for Level 2a.

An example file header is given in **Section 3.3.5.**

The final XCO2 product is contained in the following columns:

```
# Col37: XCO2          : XCO2 [ppm]
# Col38: XCO2_err      : XCO2 error [%]
…
# Col47: XCO2FQ        : XCO2 final quality flag (0:good 1:bad)
```

Column 47 which contains the final XCO2 quality flag comes from / is identical with the final quality flag contained in the Level 2a wasaux file.

3.4.6 Product description: XCO2 Level3_monthly_grid_QUALgood

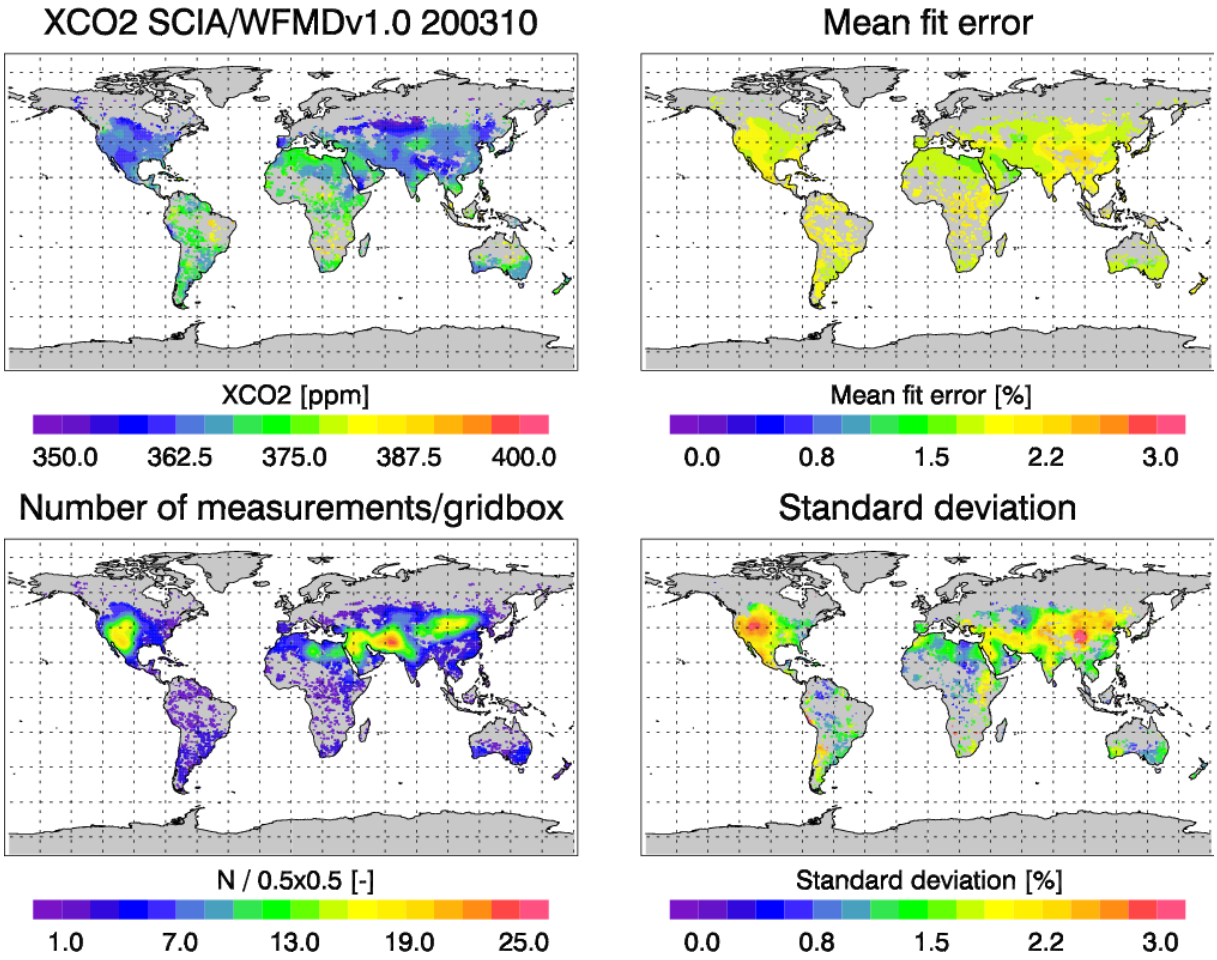
This data product contains the gridded data (0.5 deg latitude x 0.5 deg longitude) at monthly resolution produced from the corresponding Level 2b file.

Each (ASCII) file contains a header followed by a matrix of data.

The file name extension is “grid”.

The structure of the XCO2 grid files is identical with the structure of the CO column data product grid files described in **Section 3.2.6**.

Here the content of the grid files for October 2003:



4 References

A full reference list including latest updates and links to PDF files of the papers is given here:

http://www.iup.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/wfmd_references.html

Buchwitz, M., I. Khlystova, H. Bovensmann, J. P. Burrows, Three years of global carbon monoxide from SCIAMACHY: Comparison with MOPITT and first results related to the detection of enhanced CO over cities, Atmos. Chem. Phys., 7, 2399-2411, 2007a.

Buchwitz, M., O. Schneising, J. P. Burrows, H. Bovensmann, M. Reuter, J. Notholt, First direct observation of the atmospheric CO2 year-to-year increase from space, Atmos. Chem. Phys., 7, 4249-4256, 2007b.

Buchwitz, M., I. Khlystova, O. Schneising, H. Bovensmann, J. P. Burrows, SCIAMACHY/WFM-DOAS tropospheric CO, CH_4, and CO_2 scientific data products: Validation and recent developments, *in proceedings of* Third Workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-3), 4-7 Dec. 2006, ESA/ESRIN, Frascati, Italy, ESA Publications Division Special Publication SP-642 (CD), 2006b.

Buchwitz, M., R. de Beek, S. Noël, J. P. Burrows, H. Bovensmann, O. Schneising, I. Khlystova, M. Bruns, H. Bremer, P. Bergamaschi , S. Körner, and M. Heimann, Atmospheric carbon gases retrieved from SCIAMACHY by WFM-DOAS: version 0.5 CO and CH_4 and impact of calibration improvements on CO_2 retrieval, Atmos. Chem. Phys., 6, 2727-2751, 2006a.

Buchwitz, M., R. de Beek, S. Noël, J. P. Burrows, H. Bovensmann, H. Bremer, P. Bergamaschi, S. Körner, M. Heimann, Carbon monoxide, methane and carbon dioxide columns retrieved from SCIAMACHY by WFM-DOAS: year 2003 initial data set, Atmos. Chem. Phys., 5, 3313-3329, 2005b.

Buchwitz, M., R. de Beek, J. P. Burrows, H. Bovensmann, T. Warneke, J. Notholt, J. F. Meirink, A. P. H. Goede, P. Bergamaschi, S. Körner, M. Heimann, and A. Schulz, Atmospheric methane and carbon dioxide from SCIAMACHY satellite data: Initial comparison with chemistry and transport models, Atmos. Chem. Phys., 5, 941-962, 2005a.

Buchwitz, M., R. de Beek, K. Bramstedt, S. Noël, H. Bovensmann, and J. P. Burrows, Global carbon monoxide as retrieved from SCIAMACHY by WFM-DOS, Atmos. Chem. Phys., 4, 1954-1960, 2004.

Buchwitz, M., and John P. Burrows, Retrieval of CH4, CO, and CO2 total column amounts from SCIAMACHY near-infrared nadir spectra: Retrieval algorithm and first results, Proceedings of SPIE 5235, Remote Sensing of Clouds and the Atmosphere VIII, K. P. Schäfer and A. Comeron and M. R. Carleer and R. H. Picard (Editors), 375-388, 2004.

Buchwitz, M., V.V. Rozanov, and J.P. Burrows, A near-infrared optimized DOAS method for the fast global retrieval of atmospheric CH_4, CO, CO_2, H_2O, and N_2O total column amounts from SCIAMACHY Envisat-1 nadir radiances, J. Geophys. Res. 105, 15,231-15,245, 2000b.

Buchwitz, M., V.V. Rozanov, and J.P. Burrows, A correlated-*k* distribution scheme for overlapping gases suitable for retrieval of atmospheric constituents from moderate resolution radiance measurements in the visible/near-infrared spectral region, J. Geophys. Res. 105, 15,247-15,261, 2000a.

Dils, B., M. De Mazière, T. Blumenstock, F. Hase, I. Kramer, E. Mahieu, P. Demoulin, P. Duchatelet, J. Mellqvist, A. Strandberg, M. Buchwitz, I. Khlystova, O. Schneising, V. Velazco, J. Notholt, R. Sussmann, W. Stremme, Validation of WFM-DOAS v0.6 CO and v1.0 CH_4 scientific products using European ground-based FTIR measurements, *in proceedings of* Third Workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-3), 4-7 Dec. 2006, ESA/ESRIN, Frascati, Italy, ESA Publications Division Special Publication SP-642 (CD), 2006b.

Dils, B., M. De Mazière, J. F. Müller, T. Blumenstock, M. Buchwitz, R. de Beek, P. Demoulin, P. Duchatelet, H. Fast, C. Frankenberg, A. Gloudemans, D. Griffith, N. Jones, T. Kerzenmacher, E. Mahieu, J. Mellqvist, S. Mikuteit, R. L. Mittermeier, J. Notholt, H. Schrijver, D. Smale, A. Strandberg, W. Stremme, K. Strong, R. Sussmann, J. Taylor, M. van den Broek, T. Warneke, A. Wiacek, S. Wood, Comparisons between SCIAMACHY and ground-based FTIR data for total columns of CO, CH_4, CO_2 and N_2O, Atmos. Chem. Phys., 6, 1953-1967, 2006a.

Schneising, O., Buchwitz, M., Burrows, J. P., Bovensmann, H., Reuter, M., Notholt, J., Macatangay, R., and Warneke, T., Three years of greenhouse gas column-averaged dry air mole fractions retrieved from satellite - Part 1: Carbon dioxide, Atmos. Chem. Phys., 8, 3827-3853, 2008.

Schneising, O., Buchwitz, M., Burrows, J. P., Bovensmann, H., Bergamaschi, P., and Peters, W., Three years of greenhouse gas column-averaged dry air mole fractions retrieved from satellite - Part 2: Methane, Atmos. Chem. Phys., 9, 443-465, 2009.

Khlystova, I., Buchwitz, M., Burrows, J. P., Bovensmann, H., and Fowler, D., Carbon monoxide spatial gradients over source regions as observed by SCIAMACHY: A case study for the United Kingdom, Advances in Space Research, 43, 923-929, doi: 10.1016/j.asr.2008.10.012, 2009.

Sussmann, R., M. Buchwitz, Initial validation of ENVISAT/SCIAMACHY columnar CO by FTIR profile retrievals at the Ground-Truthing Station Zugspitze, Atmos. Chem. Phys., 5, 1497-1503, 2005.

Sussmann, R., W. Stremme, M. Buchwitz, R. de Beek, Validation of ENVISAT/SCIAMACHY columnar methane by solar FTIR spectrometry at the Ground-Truthing Station Zugspitze, Atmos. Chem. Phys., 5, 2419-2429, 2005.

Warneke, T., de Beek, R., Buchwitz, M., Notholt, J., Schulz, A., Velazco, V., and Schrems, O., Shipborne solar absorption measurements of CO_2, CH_4, N_2O, and CO and comparison the SCIAMACHY WFM-DOAS retrievals, Atmos. Chem. Phys., 5, 2029-2034, 2005.