ESA Climate Change Initiative “Plus” (CCI+)

Product User Guide (PUG)

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TROPOMI WFM-DOAS XCH_4

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

Written by:

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Version Nr.	Date	Status	Reason for change
Version 1	23 Oct 2019	Final	New document
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Product User Guide (PUG)

TROPOMI WFM-DOAS (TROPOMI/WFMD) XCH_4

Prepared by:

Oliver Schneising

Valid for:

TROPOMI WFM-DOAS

Product	**Version**
Methane column-averaged dry air mole fraction (XCH_4)	v1.2

Contents

Spectrometer	SWIR	
Band ID	7	8
Spectral Range [nm]	2300 – 2343	2343 – 2389
Spectral Resolution FWHM [nm]	0.227	0.225
Spectral Sampling [nm]	0.094	
Spatial Sampling [km^2]	7.1×7.5	
Detector Binning Factor	1	

Table 1: Summary of the TROPOMI SWIR spectral bands and their key features (Rozemeijer and Kleipool, 2018).

1 Purpose of document

This document describes the TROPOMI WFM-DOAS (TROPOMI/WFMD) XCH_4 data product and illustrates how to use it.

2 Introduction

2.1 The TROPOMI instrument on Sentinel-5 Precursor

The TROPOspheric Monitoring Instrument (TROPOMI) is a spaceborne nadir viewing spectrometer with bands in the ultraviolet and visible (270-495 nm), the near infrared (675-775 nm) and the shortwave infrared (2305-2385 nm) (Veefkind et al., 2012). TROPOMI combines daily global coverage with a high spatial resolution in order to focus on the troposphere where concentrations of trace gas and aerosol species rapidly change. Light from different wavelength bands is measured by TROPOMI to generate various data products. Some of the species measured by TROPOMI include ozone, nitrogen dioxide, methane, and carbon monoxide.

Sentinel-5P was launched in October 2017 into a sun-synchronous orbit with an equator crossing time of 13:30. TROPOMI's observations of overtone absorptions in the shortwave infrared (SWIR) solar backscattered spectrum yield the vertical columns of CH_4 with high sensitivity down to the Earth's surface (Schneising et al., 2019). The instrument has a wide swath of 2600 km consisting of single measurements with a horizontal resolution of typically $7 \times 7\,km^2$ in the SWIR bands. The characteristics of the TROPOMI SWIR bands are summarised in Table 1.

2.2 The WFM-DOAS retrieval algorithm

The Weighting Function Modified Differential Optical Absorption Spectroscopy (WFM-DOAS) algorithm (Buchwitz et al., 2005a,b; Schneising et al., 2008, 2009, 2011, 2012; Heymann et al., 2012a,b; Schneising et al., 2013, 2014a,b, 2019, 2020a,b) is a least-squares method based on scaling (or shifting) pre-selected atmospheric vertical profiles. The column-averaged dry air mole fractions of methane (denoted XCH_4) are derived from the vertical column amounts of CH_4 by normalising with the dry air column, which is obtained from the European Centre for Medium-Range Weather Forecasts (ECMWF) analysis. The corresponding vertical columns of CH_4 are retrieved from the measured sun-normalised radiance using spectral fitting windows in the SWIR spectral region (2311-2315.5 nm and 2320-2338 nm).

The global distribution of the retrieved mole fractions XCH_4 for the years 2018 and 2019 is shown in Figure 1. Clearly visible is the interhemispheric gradient with larger methane concentrations on the northern hemisphere, where the majority of sources is located, superimposed by enhancements over prominent source regions like anthropogenic emissions from fossil fuels and rice cultivation in China, India, and Southeast Asia. Other visible source regions include tropical wetlands as well as anthropogenic emissions in California or the Padan Plain in Italy.

From the validation with ground-based Fourier Transform Spectroscopy (FTS) measurements of the Total Carbon Column Observing Network (TCCON) (Wunch et al., 2011) at the 24 TCCON sites listed in Table 2, realistic error estimates of the satellite data are provided and summarised in Table 3. For the sake of completeness, the error characteristics of XCO, which is simultaneously retrieved with XCH_4 and also included in the product, are also quoted.

3 Product description

The data product is based on TROPOMI Level 1b V01.00.00 files comprising spectra from the nominal operational mode, which started end of April 2018, and reprocessed spectra from the previous six-month commissioning phase.

3.1 Product content and format

The CH4-TROPOMI-WFMD data products are stored per day in seperate NetCDF-files (NetCDF-4 classic model). The product files contain the key product, i.e. the

Station	Latitude [°]	Longitude [°]	Altitude [km]	Reference
Eureka	80.05	−86.42	0.61	Strong et al. (2019)
Ny-Ålesund	78.92	11.92	0.02	Notholt et al. (2017)
Sodankylä	67.37	26.63	0.19	Kivi et al. (2014)
East Trout Lake	54.35	−104.99	0.50	Wunch et al. (2018)
Białystok	53.23	23.03	0.19	Deutscher et al. (2015)
Bremen	53.10	8.85	0.03	Notholt et al. (2014)
Karlsruhe	49.10	8.44	0.11	Hase et al. (2015)
Paris	48.85	2.36	0.06	Te et al. (2014)
Orléans	47.97	2.11	0.13	Warneke et al. (2014)
Garmisch	47.48	11.06	0.75	Sussmann and Rettinger (2018)
Park Falls	45.94	−90.27	0.44	Wennberg et al. (2017)
Rikubetsu	43.46	143.77	0.38	Morino et al. (2018c)
Lamont	36.60	−97.49	0.32	Wennberg et al. (2016b)
Tsukuba	36.05	140.12	0.03	Morino et al. (2018a)
Edwards	34.96	−117.88	0.70	Iraci et al. (2016)
JPL	34.20	−118.18	0.39	Wennberg et al. (2016a)
Caltech	34.14	−118.13	0.24	Wennberg et al. (2015)
Saga	33.24	130.29	0.01	Shiomi et al. (2014)
Burgos	18.53	120.65	0.04	Morino et al. (2018b)
Ascension Island	−7.92	−14.33	0.03	Feist et al. (2014)
Darwin	−12.46	130.93	0.04	Griffith et al. (2014a)
Réunion	−20.90	55.49	0.09	De Mazière et al. (2017)
Wollongong	−34.41	150.88	0.03	Griffith et al. (2014b)
Lauder	−45.04	169.68	0.37	Sherlock et al. (2014)

Table 2: TCCON sites used in the validation ordered according to latitude from north to south.

	XCH_4 [ppb]	XCO [ppb]
Global Offset	0.55	5.47
Random Error	14.28	5.27
Systematic Error (spatio-temporal)	4.50	2.04

Table 3: Error characterisation of the WFM-DOAS data products (valid for TROPOMI/WFMD v1.2 XCH_4 and XCO).

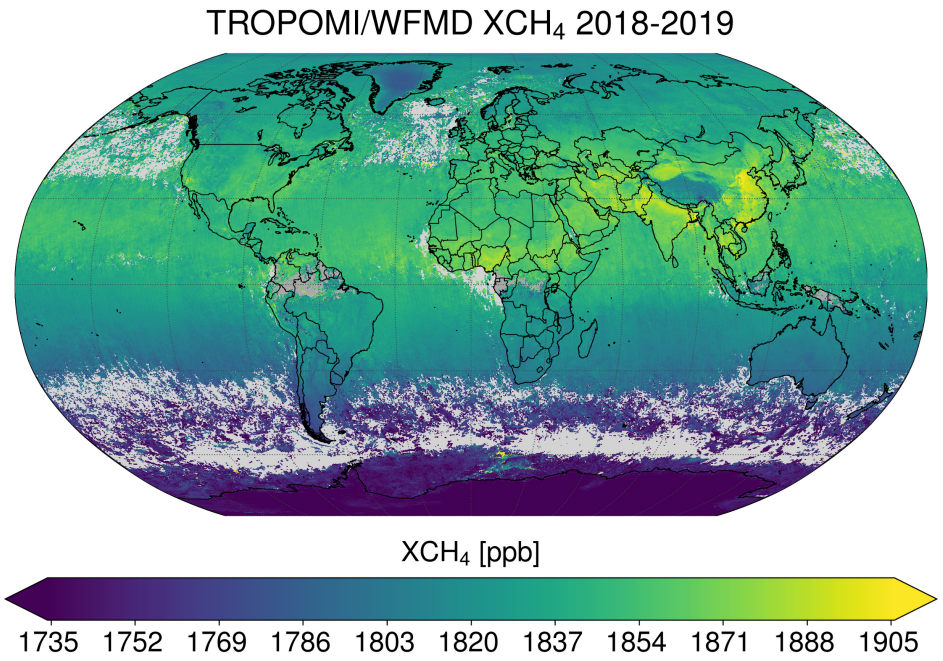

Figure 1: Biennial mean (2018-2019) of retrieved TROPOMI/WFMD v1.2 methane.

retrieved column-averaged dry air mole fractions XCH_4, as well as the column-averaged dry air mole fractions XCO and several other useful parameters (see Section 3.5 for details). Information relevant for the use of the data is also included in the data file, e.g. the averaging kernels.

3.2 Data usage

The column-averaged dry air mole fractions of methane are stored in the variable `xch4` in the NetCDF product files `ESACCI-GHG-L2-CH4-CO-TROPOMI-WFMD-YYYYMMDD-fv1.nc` (see Section 3.5).

If the data are to be compared with other data for which vertical profile information is available (e.g. comparison to models), the column averaging kernels should be applied to the model profiles using the formula

$$X_{\text{mod}} = \sum_l \left(X^l_{\text{apr}} + A_l (X^l_{\text{mod}} - X^l_{\text{apr}}) \right) w_l \qquad (1)$$

where l is the index of the vertical layer, A_l the averaging kernel (variables `xch4_averaging_kernel` and `xco_averaging_kernel` in NetCDF product files), X^l_{apr} the a-priori mole fraction (variables `ch4_profile_apriori` and

`co_profile_apriori` in product files) and X^l_{mod} the simulated mole fraction of layer l. w_l is the layer dependent pressure weight (variable `pressure_weight` in product files).

3.3 Tools for reading the data

The data are stored in NetCDF format (NetCDF-4 classic model) which can be read with standard tools in the common programming languages (Python, IDL, Matlab, Fortran90, C++, etc).

3.4 Known limitations and issues

The file names `ESACCI-GHG-L2-CH4-CO-TROPOMI-WFMD-YYYYMMDD-fv1.nc` deviate slighty from the GHG-CCI file naming convention to take into a account that a comprehensive carbon monoxide mole fraction data set is also included in the product. For the same reason, the variable of the common quality flag (for XCH_4 and XCO) is simply named `quality_flag`, differing from the harmonised convention `xch4_quality_flag` introduced in the GHG-CCI Product Specification Document. For the sake of consistency, the corresponding variables will be named `xch4_quality_flag` and `xco_quality_flag` in future versions even if the flags are identical.

The reported uncertainties σ (included product variables `xch4_uncertainty` and `xco_uncertainty`) are too optimistic because they only comprise the propagated measurement errors given in the Level 1 files and neglect the (unknown) pseudo-noise component determined by specific atmospheric parameters or instrumental features (e.g., potential striping in flight direction due to different offsets and gains of pixels of the detector array used for the staring push-broom concept of TROPOMI). If the uncertainties are of concern for the intended application, more realistic uncertainty estimates $\hat{\sigma}$ are obtained by applying these error parameterisations obtained from a comparison of the reported uncertainties with the measured scatter relative to the TCCON:

$$\hat{\sigma}_{XCH_4} = 1.37 \cdot \sigma_{XCH_4} + 7.78\,\text{ppb} \quad (2)$$

$$\hat{\sigma}_{XCO} = 0.9 \cdot \sigma_{XCO} + 3\,\text{ppb} \quad (3)$$

Corresponding error parameterisations will be explicitly implemented in the next version of the product, so that the variables `xch4_uncertainty` and `xco_uncertainty`) can be used directly in future versions.

3.5 Data file content

The structure of the Level2 product files `ESACCI-GHG-L2-CH4-CO-TROPOMI-WFMD-YYYYMMDD-fv1.nc` is summarised in the following:

```
netcdf ESACCI-GHG-L2-CH4-CO-TROPOMI-WFMD-20180701-fv1 {
dimensions:
    sounding_dim = 400775 ;
    level_dim = 21 ;
    layer_dim = 20 ;
    corners_dim = 4 ;
variables:
    double time(sounding_dim) ;
       time:standard_name = "time" ;
       time:long_name = "time" ;
       time:units = "seconds since 1970-01-01 00:00:00" ;
       time:calendar = "standard" ;
    float latitude(sounding_dim) ;
       latitude:standard_name = "latitude" ;
       latitude:long_name = "latitude" ;
       latitude:units = "degree_north" ;
       latitude:valid_range = -90.f, 90.f ;
       latitude:comment = "Center latitude of the measurement" ;
    float longitude(sounding_dim) ;
       longitude:standard_name = "longitude" ;
       longitude:long_name = "longitude" ;
       longitude:units = "degree_east" ;
       longitude:valid_range = -180.f, 180.f ;
       longitude:comment = "Center longitude of the measurement" ;
    float solar_zenith_angle(sounding_dim) ;
       solar_zenith_angle:standard_name = "solar_zenith_angle" ;
       solar_zenith_angle:long_name = "solar zenith angle" ;
       solar_zenith_angle:units = "degree" ;
       solar_zenith_angle:comment = "Solar zenith angle is the the angle between the
                line of sight to the sun and the local vertical." ;
    float sensor_zenith_angle(sounding_dim) ;
       sensor_zenith_angle:standard_name = "sensor_zenith_angle" ;
       sensor_zenith_angle:long_name = "sensor zenith angle" ;
       sensor_zenith_angle:units = "degree" ;
       sensor_zenith_angle:comment = "Sensor zenith angle is the angle between the line
                of sight to the sensor and the local vertical." ;
    float azimuth_difference(sounding_dim) ;
       azimuth_difference:long_name = "azimuth difference" ;
       azimuth_difference:units = "degree" ;
       azimuth_difference:comment = "Relative azimuth angle between sun and sensor
                direction." ;
    float xch4(sounding_dim) ;
       xch4:standard_name = "dry_atmosphere_mole_fraction_of_methane" ;
       xch4:long_name = "column-averaged dry air mole fraction of atmospheric methane" ;
       xch4:units = "1e-9" ;
       xch4:comment = "Retrieved column-averaged dry air mole fraction of atmospheric
                methane (XCH4) in ppb" ;
    float xch4_uncertainty(sounding_dim) ;
       xch4_uncertainty:long_name = "1-sigma uncertainty of the retrieved column-averaged
                dry air mole fraction of atmospheric methane" ;
       xch4_uncertainty:units = "1e-9" ;
       xch4_uncertainty:comment = "1-sigma uncertainty of the retrieved column-averaged
                dry air mole fraction of atmospheric methane (XCH4) in ppb" ;
    float xco(sounding_dim) ;
```

```
   xco:long_name = "column-averaged dry air mole fraction of atmospheric
            carbon monoxide" ;
   xco:units = "1e-9" ;
   xco:comment = "Retrieved column-averaged dry air mole fraction of atmospheric
            carbon monoxide (XCO) in ppb" ;
float xco_uncertainty(sounding_dim) ;
   xco_uncertainty:long_name = "1-sigma uncertainty of the retrieved column-averaged
            dry air mole fraction of atmospheric carbon monoxide" ;
   xco_uncertainty:units = "1e-9" ;
   xco_uncertainty:comment = "1-sigma uncertainty of the retrieved column-averaged
            dry air mole fraction of atmospheric carbon monoxide (XCO) in ppb" ;
int quality_flag(sounding_dim) ;
   quality_flag:long_name = "quality flag" ;
   quality_flag:flag_values = 0, 1 ;
   quality_flag:flag_meanings = "good_quality potentially_bad_quality" ;
   quality_flag:comment = "0=good, 1=bad" ;
float pressure_levels(sounding_dim, level_dim) ;
   pressure_levels:long_name = "pressure levels" ;
   pressure_levels:units = "hPa" ;
   pressure_levels:comment = "Pressure levels define the boundaries of the
            averaging kernel and a priori profile layers.\n",
           "Levels are ordered from surface to top of atmosphere." ;
float pressure_weight(sounding_dim, layer_dim) ;
   pressure_weight:long_name = "pressure weight" ;
   pressure_weight:units = "1" ;
   pressure_weight:comment = "Layer dependent weights needed to apply the
            averaging kernels." ;
float ch4_profile_apriori(sounding_dim, layer_dim) ;
   ch4_profile_apriori:long_name = "a priori dry air mole fraction profile of
            atmospheric methane" ;
   ch4_profile_apriori:units = "1e-9" ;
   ch4_profile_apriori:comment = "A priori dry-air mole fraction profile of
            atmospheric methane in ppb.\n",
           "All values represent layer averages within the corresponding pressure
            levels. Profiles are ordered from surface to top of atmosphere." ;
float xch4_averaging_kernel(sounding_dim, layer_dim) ;
   xch4_averaging_kernel:long_name = "xch4 averaging kernel" ;
   xch4_averaging_kernel:units = "1" ;
   xch4_averaging_kernel:comment = "Represents the altitude sensitivity of the
            retrieval as a function of pressure.\n",
           "All values represent layer averages within the corresponding pressure levels.\n",
           "Profiles are ordered from surface to top of atmosphere." ;
float co_profile_apriori(sounding_dim, layer_dim) ;
   co_profile_apriori:long_name = "a priori dry air mole fraction profile of
            atmospheric carbon monoxide" ;
   co_profile_apriori:units = "1e-9" ;
   co_profile_apriori:comment = "A priori dry-air mole fraction profile of
            atmospheric carbon monoxide in ppb.\n",
           "All values represent layer averages within the corresponding pressure
            levels. Profiles are ordered from surface to top of atmosphere." ;
float xco_averaging_kernel(sounding_dim, layer_dim) ;
   xco_averaging_kernel:long_name = "xco averaging kernel" ;
   xco_averaging_kernel:units = "1" ;
   xco_averaging_kernel:comment = "Represents the altitude sensitivity of the
            retrieval as a function of pressure.\n",
           "All values represent layer averages within the corresponding pressure levels.\n",
           "Profiles are ordered from surface to top of atmosphere." ;
int orbit_number(sounding_dim) ;
   orbit_number:long_name = "orbit number" ;
   orbit_number:units = "1" ;
```

```
      orbit_number:comment = "Orbit number" ;
   int scanline(sounding_dim) ;
      scanline:long_name = "along track dimension index" ;
      scanline:units = "1" ;
      scanline:comment = "This dimension variable defines the indices along track" ;
   int ground_pixel(sounding_dim) ;
      ground_pixel:long_name = "across track dimension index" ;
      ground_pixel:units = "1" ;
      ground_pixel:comment = "This dimension variable defines the indices across track" ;
   float latitude_corners(sounding_dim, corners_dim) ;
      latitude_corners:long_name = "latitude_corners" ;
      latitude_corners:units = "degree_north" ;
      latitude_corners:valid_range = -90.f, 90.f ;
      latitude_corners:comment = "Corner latitudes of the measurement" ;
   float longitude_corners(sounding_dim, corners_dim) ;
      longitude_corners:long_name = "longitude_corners" ;
      longitude_corners:units = "degree_east" ;
      longitude_corners:valid_range = -180.f, 180.f ;
      longitude_corners:comment = "Corner longitudes of the measurement" ;
   float altitude(sounding_dim) ;
      altitude:standard_name = "altitude" ;
      altitude:long_name = "altitude" ;
      altitude:units = "m" ;
      altitude:comment = "Average surface altitude" ;
   float apparent_albedo(sounding_dim) ;
      apparent_albedo:long_name = "apparent surface albedo" ;
      apparent_albedo:units = "1" ;
      apparent_albedo:comment = "Retrieved surface albedo at 2313nm" ;
   int land_fraction(sounding_dim) ;
      land_fraction:long_name = "land fraction" ;
      land_fraction:units = "1e-2" ;
      land_fraction:valid_range = 0, 100 ;
      land_fraction:comment = "Land fraction of the observed scene in percent" ;
   float cloud_parameter(sounding_dim) ;
      cloud_parameter:long_name = "cloud parameter from strong water vapour absorption" ;
      cloud_parameter:units = "1" ;
      cloud_parameter:comment = "Ratio of measured to cloud-free reference radiance
               for selected strong water vapour lines" ;
   float h2o_column(sounding_dim) ;
      h2o_column:long_name = "vertical column of water vapour" ;
      h2o_column:units = "g cm-2" ;
      h2o_column:comment = "Retrieved vertical column amount of water vapour" ;
   float h2o_column_uncertainty(sounding_dim) ;
      h2o_column_uncertainty:long_name = "1-sigma uncertainty of the retrieved vertical
               column of atmospheric water vapour" ;
      h2o_column_uncertainty:units = "g cm-2" ;
      h2o_column_uncertainty:comment = "1-sigma uncertainty of the retrieved vertical
               column of atmospheric water vapour" ;

// global attributes:
   :title = "TROPOMI/WFMD XCH4 and XCO" ;
   :institution = "University of Bremen" ;
   :source = "TROPOMI L1B version 01.00.00" ;
   :history = "2019 - product generated with WFMD" ;
   :tracking_id = "a828ddf9-4c4f-4419-9500-a06cbf2e0f05" ;
   :Conventions = "CF-1.6" ;
   :product_version = "v1.2" ;
   :summary = "Weighting Function Modified DOAS (WFMD) was adjusted to simultaneously
            retrieve column-averaged dry air mole fractions of atmospheric methane and
            carbon monoxide from the shortwave-infrared (SWIR) nadir spectra of the
```

```
            TROPOMI instrument onboard Sentinel-5 Precursor." ;
    :keywords = "satellite, Sentinel-5 Precursor, TROPOMI, atmosphere, methane, carbon monoxide" ;
    :id = "ESACCI-GHG-L2-CH4-CO-TROPOMI-WFMD-20180701-fv1.nc" ;
    :naming_authority = "iup.uni-bremen.de" ;
    :keywords_vocabulary = "NASA Global Change Master Directory (GCMD)" ;
    :cdm_data_type = "point" ;
    :comment = "These data were produced at the University of Bremen in the framework
            of the ESA GHG-CCI project" ;
    :date_created = "20190530T225016Z" ;
    :creator_name = "University of Bremen, IUP, Oliver Schneising" ;
    :creator_email = "schneising@iup.physik.uni-bremen.de" ;
    :project = "Climate Change Initiative - European Space Agency" ;
    :geospatial_lat_min = -90 ;
    :geospatial_lat_max = 90 ;
    :geospatial_lat_units = "degree_north" ;
    :geospatial_lon_min = -180 ;
    :geospatial_lon_max = 180 ;
    :geospatial_lon_units = "degree_east" ;
    :geospatial_vertical_min = 0 ;
    :geospatial_vertical_max = 100000 ;
    :time_coverage_start = "20180701T000000Z" ;
    :time_coverage_end = "20180701T235959Z" ;
    :time_coverage_duration = "P1D" ;
    :time_coverage_resolution = "P1D" ;
    :standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Conventions
                Version 1.6" ;
    :license = "ESA CCI Data Policy: free and open access" ;
    :platform = "Sentinel-5 Precursor" ;
    :sensor = "TROPOMI" ;
    :spatial_resolution = "7km x 7km at nadir (typically)" ;
}
```

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