SRON RemoTeC-S5P scientific XCH_4 data product Product User Guide

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1 Introduction

This document presents the SRON RemoTeC-S5P XCH_4 [1] scientific product, version 17, available to download at the SRON ftp site[2]. This product is processed as part of the operational algorithm development activities. This document does not include information that overlaps with the operational ATBD and other official documentation (PRF, PUG) that should be also considered as a reference when using the TROPOMI CH_4 data (see Sect. 3).

This document describes the most important characteristics of the SRON RemoTeC-S5P CH_4 scientific product with respect to the operational TROPOMI-S5P CH_4 product. This document intends to serve as a guide to the user of the SRON RemoTeC-S5P CH_4 scientific product, given the differences that exist with respect to the operational product in terms of format and algorithm settings.

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1.1 SRON RemoTeC-S5P XCH_4 scientific product

The CH_4 total column-average dry-air mole fraction (XCH_4) retrieved from TROPOMI with the operational retrieval algorithm largely complies with the mission requirement of precision and accuracy below 1%. Updates that further improved the quality of the data were implemented in the operational processing in July 2021 (version 2.2.0, orbit 19538, see Table 2 on Product Readme File for history of processor versions), with significantly improved data quality of the bias-corrected product (Hasekamp et al. (2019), Lorente et al. (2021)). The updates relate to the regularization scheme, the selection of the spectroscopic database, and a more sophisticated a posteriori correction for the albedo dependence.

Latest developments that further improve the quality of the data are implemented in the scientific algorithm that results in the TROPOMI XCH_4 product that is the focus of this document. This updated retrieval algorithm is referred to as the SRON RemoTeC-S5P XCH_4 scientific retrieval algorithm, version 17. Our updated SRON RemoTeC-S5P XCH_4 scientific product corresponds to the version that will be implemented for use in the operational processing in November 2021 (version 2.3.1). The main update on version 17 with respect to previous version is the coverage. Version 17 includes measurements over ocean for observations made under sun-glint geometries.

The main differences between the scientific and operational products are summarized in Table 1.

2 Product description

2.1 Product content and format

In the same way as the operational product, the scientific version of the SRON RemoTeC-S5P XCH_4 product is stored per orbit in a single file that contains individual retrievals for each pixel. The file name contains the version number (i.e. 17) followed by the orbit number, e.g. 's5p_l2_ch4_<version>_<orbit_number>.nc' (e.g. s5p_l2_ch4_0017_03779.nc).

[1] XCH_4 is defined as the methane total column-average dry-air mole fraction
[2] https://ftp.sron.nl/open-access-data-2/TROPOMI/tropomi/ch4/

	SRON RemoTeC-S5P (v 17) Operational (v 2.3.1)	SRON RemoTeC-S5P (v 14) Operational (v 2.2.0)	Operational (v 1.2.0)
Coverage	Land and ocean	Land	Land
Regularization	Scattering layer altitude fixed to prior (3000 m)	Constant regularization different for XCH_4 and scattering parameters	L-Curve
Cross section	SEOM-IAS	SEOM-IAS	HITRAN 2008 + Scheepmaker et al. (2013)
Bias correction	Land: same as v 14/v 2.2.0 Ocean: correction factor	Independent B-spline fit to surface albedo	Based on GOSAT linear fit to surface albedo
Altitude DEM	SRTM 15” (v 17) GMTED2010 S5P (Oper v 2.3.1)	SRTM 15” (v 14) GMTED2010 S5P (Oper v 2.2.0)	GMTED2010 S5P
Meteorology	ECMWF reanalysis (v 17) ECMWF forecast (Oper v 2.3.1)	ECMWF reanalysis (v 14) ECMWF forecast (Oper v 2.2.0)	ECMWF forecast
Reference	Updated ATBD (Hasekamp et al, 2019)	Lorente et al. (2021)	Hu et al. (2016)

Table 1: Main differences between SRON RemoTeC S5P XCH_4 scientific product and operational version 2.2.0, 2.3.1, 1.2.0

The variables are either one dimensional (nobs, i.e. number of observations) or two dimensional if the variable is retrieved in both the near-infrarred (NIR) and short-wave infrared SWIR spectral channels (nobs, nwin with nwin = 2). This is the case of the surface albedo and the scattering parameters. The first value corresponds to the NIR band and the second one to the SWIR band. The format with only one dimension (nobs) is the most noticeable difference with respect to the operational product regarding the format of the variables (in the operational product variables are stored with across x along track dimension). In the 'instrument' group of the files all the necessary variables are provided in case the user wants to make the conversion from one format to the other: pixel_id, scanline and ground_pixel. See Sect. 2.4 for details on the file content.

The main retrieved variable is the methane total column-average dry-air mole fraction (XCH_4). In the SRON product this variable is called 'xch4' and the one with the correction applied 'xch4_corrected'. In the operational product, these two variables are named 'methane_mixing_ratio' and 'methane_mixing_ratio_bias_corrected' respectively, both stored in the 'PRODUCT' group.

Another variable that is different for the operational product is the relative azimuth angle (RAA). The SRON product contains the solar zenith angle (θ_o) and the viewing zenith angle (θ), but not the corresponding azimuths (φ_o, φ). Instead we provide the relative azimuth angle, which is a combination of both, based on the following definition:

$$RAA = |180. - |(\varphi_o - \varphi)|| \tag{1}$$

The cloud fraction variable under the 'meteo_group' contains four values, one for the inner field of view (IFOV) and another three for the outer field of view (OFOV) with a 10, 50 and 100% scaled-up of the field of view respectively.

The file does not contain the orbit date in the name, the specific date and time of the overpass is written in the 'time' variable in the 'instrument' group. The specific orbit number can also be obtained from the l1b_file variable in the 'instrument' group.

2.2 Filtering and data usage

It is recommended to use the variable ’xch4_corrected’ in the ’target_product’ group of the netCDF files. It is also recommended to use pixels with the parameter ’qa_value’ in the diagnostics group equal to 1 (i.e. qa_value == 1). A qa value of 0.4 denotes that the filtering threshold has been exceed at least for one of the variables that are used as filtering criteria. The filter settings used in the SRON product are the same as in the operational product.

The most relevant filtering criteria are:

- Cloud fraction < 0.001 (IFOV, OFOV)
- Ratio weak and strong CH_4 column 0.85 - 1.15
- Standard deviation of ratio weak and strong CH_4 column < 0.05
- Aerosol optical thickness (NIR) < 0.3
- $\chi^2 < 100$
- Solar zenith angle < 70°
- Precision < 10 ppb
- Surface roughness < 80 m
- Surface albedo (SWIR) > 0.02 (only land)

Applying the recommended qa_value == 1 includes in version 17 pixels both over land and over ocean. If users want to use only land or ocean pixels, they should include in their filtering the ‘land flag’ or ‘sun glint flag’ to select specific pixels.

2.2.1 Pre-filtering

There is a pre-filtering applied to the TROPOMI data before the processing starts. Those pixels that do not pass the pre-filtering have a qa_value of 0. The most strict pre-filter setting is related to the cloud fraction: only pixels with a cloud fraction lower than 0.02 are processed. Furthermore, there is a lower threshold for the SWIR signal-to-noise ratio of 50, a lower threshold for the fraction of ’good’ spectral pixels of 70% and a lower threshold for the surface roughness of 100 m. Pixels with a solar zenith angle higher than 75° and a viewing zenith angle of 60° are also not processed.

2.3 Data features

2.3.1 Snow covered scenes

In the validation of the TROPOMI XCH_4, it was found that during the winter XCH_4 retrieved with TROPOMI was biased high with respect to the ground based stations of the TCCON network at high latitudes (i.e. Sodankyla and East Trout Lake). This issue is discussed more in detail in Lorente et al. (AMTD, 2020).

The surface albedo retrieved both in the SWIR and NIR spectral range can be used to filter scenes covered by snow, using the so-called blended albedo (Wunch et al., 2011):

$$A_{\text{blended}} = 2.4 \cdot A_{\text{NIR}} - 1.13 \cdot A_{\text{SWIR}} < 0.85 \tag{2}$$

This filter is not applied in the default filter of the XCH_4 product, but users can apply it in their own data analysis or when using the XCH_4 data for inverse modelling studies.

2.3.2 VIIRS cloud mask update

In March 2020, orbit 12432, there was an update to the VIIRS cloud mask used to estimate the cloud coverage that is used as a filter in the XCH_4 product. The cloud mask was switched from the VICMO (or VCM) cloud mask to the Enterprise Cloud Mask (ECM). As a consequence, there was a significant decrease in the data yield due to the too stringent cloud fraction threshold used in the filtering. In the new cloud mask, there is a significant clear scenes that are classified as probably clear. Thus, the cloud fraction definition has been adapted to also include the pixels classified as 'probably clear' together with the 'confidently clear'.

2.3.3 Cloudy data not filtered

In version 14 of the SRON RemoTeC-S5P XCH4 scientific product, some cloudy data was not filtered properly. This resulted in unrealistically low CH4 values for some scenes classified with qa_value == 1. The cloud fraction variable for these specific scenes contains NaNs or fill values, so the user can avoid using these scenes by adding an extra filtering criteria in the cloud fraction parameter just allowing valid numbers. This issue has been resolved in version 17.

2.3.4 Known artifacts

The quality of both operational and scientific data produced with RemoTeC retrieval algorithm has extensively been assessed by validation studies, as well as demonstrated by the quantification of emissions from multiple sources using TROPOMI XCH4. However, there are few known artifacts for which the origin is still under investigation. Typically these features show a clear one-to-one correlation with either the retrieved surface albedo or scattering parameters (e.g., AOD), and they might be constant in time (e.g., Barré et al. (2021)). If these particular characteristics are found when analyzing CH_4 signals, users should perform a thorough analysis to discard any possible artifacts.

2.3.5 Negative surface albedo over ocean

The retrieved surface albedo over ocean for sun-glint measurements might be lower than zero (i.e., negative values). This is because ocean measurements use a different reflectance model than that over land. Therefore, retrieved surface albedo over ocean does not have the same physical meaning as that over land.

2.4 Data file content

The data are stored in netCDF format, which can be read using standard tools from the different programming languages. The structure of the product files s5p_l2_ch4_0014_<orbit_number>.nc is summarised in the following:

```
   netcdf s5p_l2_ch4_0017_03779 {
dimensions:
```

```
    nobs = 697675 ;
   nwin = 2 ;
   nlayer = 12 ;
   nlevel = 13 ;
   ntime = 7 ;
   nchar = 299 ;
   ncorner = 4 ;
   nfov = 4 ;


global attributes:
          :title = "S5P L2 CH4 product" ;
         :institution = "SRON Netherlands Institute for Space Research" ;
         :source = "RemoTeC retrieval algorithm" ;
         :date_created = "20211009T164828" ;


group:  instrument {
 variables:
    char l1b_file(nchar) ;
   int pixel_id(nobs) ;
   int scanline(nobs) ;
   int ground_pixel(nobs) ;
   int time(nobs, ntime) ;
   float solar_zenith_angle(nobs) ;
   float viewing_zenith_angle(nobs) ;
   float relative_azimuth_angle(nobs) ;
   float latitude_center(nobs) ;
   float longitude_center(nobs) ;
   float latitude_corners(nobs, ncorner) ;
   float longitude_corners(nobs, ncorner) ;
   int glintflag(nobs) ;
   } // group instrument


group:  meteo {
 variables:
    float altitude_levels(nobs, nlevel) ;
         altitude_levels:units = "m" ;
   float surface_altitude(nobs) ;
         surface_altitude:units = "m" ;
   float surface_altitude_stdv(nobs) ;
         surface_altitude_stdv:units = "m" ;
   float dp(nobs) ;
         dp:units = "hPa" ;
   float surface_pressure(nobs) ;
         surface_pressure:units = "hPa" ;
   float dry_air_subcolumns(nobs, nlayer) ;
         dry_air_subcolumns:units = "molecules cm-2" ;
```

```
    int landflag(nobs) ;
    float u10(nobs) ;
    float v10(nobs) ;
    float fluorescence_apriori(nobs) ;
          fluorescence_apriori:units = "photons s-1 cm-2 nm-1 sr-1" ;
    float cloud_fraction(nobs, nfov) ;
    float weak_h2o_column(nobs) ;
          weak_h2o_column:units = "molecules cm-2" ;
    float strong_h2o_column(nobs) ;
          strong_h2o_column:units = "molecules cm-2" ;
    float weak_ch4_column(nobs) ;
          weak_ch4_column:units = "molecules cm-2" ;
    float strong_ch4_column(nobs) ;
          strong_ch4_column:units = "molecules cm-2" ;
    float cirrus_reflectance(nobs) ;
    float stdv_h2o_ratio(nobs) ;
          stdv_h2o_ratio:units = "molecules cm-2" ;
    float stdv_ch4_ratio(nobs) ;
          stdv_ch4_ratio:units = "molecules cm-2" ;
    } // group meteo


group:  target_product {
 variables:
     float xch4(nobs) ;
          xch4:units = "ppb" ;
    float xch4_precision(nobs) ;
          xch4_precision:units = "ppb" ;
    float xch4_column_averaging_kernel(nobs, nlayer) ;
    float ch4_profile_apriori(nobs, nlayer) ;
          ch4_profile_apriori:units = "molecules cm-2" ;
    float xch4_apriori(nobs) ;
          xch4_apriori:units = "ppb" ;
    float xch4_corrected(nobs) ;
          xch4_corrected:units = "ppb" ;
    } // group target_product


group:  side_product{
 variables:
     float fluorescence(nobs) ;
          fluorescence:units = "photons s-1 cm-2 nm-1 sr-1" ;
    float co_column(nobs) ;
          co_column:units = "molecules cm-2" ;
    float co_column_precision(nobs) ;
          co_column_precision:units = "molecules cm-2" ;
    float h2o_column(nobs) ;
          h2o_column:units = "molecules cm-2" ;
    float h2o_column_precision(nobs) ;
```

```
        h2o_column_precision:units = "molecules cm-2" ;
    float spectral_shift(nobs, nwin) ;
        spectral_shift:units = "nm" ;
    float aerosol_size(nobs) ;
    float aerosol_size_precision(nobs) ;
    float aerosol_column(nobs) ;
        aerosol_column:units = "cm-2" ;
    float aerosol_column_precision(nobs) ;
        aerosol_column_precision:units = "cm-2" ;
    float aerosol_altitude(nobs) ;
        aerosol_altitude:units = "m" ;
    float aerosol_altitude_precision(nobs) ;
        aerosol_altitude_precision:units = "m" ;
    float aerosol_optical_thickness(nobs, nwin) ;
    float surface_albedo(nobs, nwin) ;
    float surface_albedo_precision(nobs, nwin) ;
    float reflectance_max(nobs, nwin) ;
    } // group side_product


  group:  diagnostics {
   variables:
     int processing_quality_flags(nobs) ;
    int convergence(nobs) ;
    int error_id(nobs) ;
    int iterations(nobs) ;
    float chi_squared(nobs) ;
    float chi_squared_band(nobs, nwin) ;
    int number_of_spectral_points_in_retrieval(nobs, nwin) ;
    float degrees_of_freedom(nobs) ;
    float degrees_of_freedom_ch4(nobs) ;
    float degrees_of_freedom_aerosol(nobs) ;
    float signal_to_noise_ratio(nobs, nwin) ;
    float rms(nobs) ;
    float qa_value(nobs) ;
    } // group diagnostics
}
```

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