



# Algorithm Theoretical Basis Document (ATBD) – ANNEX C for product CH4\_GO2\_SRPR (v2.0.0, 2019-2021)

## C3S2\_312a\_Lot2\_DLR – Atmosphere

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## History of modifications

Version	Date	Description of modification	Chapters / Sections
1.1	20-October-2017	New document for data set CDR1 (2009-2016)	All
2.0	4-October-2018	Update for CDR2 (2009-2017)	All
3.0	12-August-2019	Update for CDR3 (2009-2018)	All
3.1	03-November-2019	Update after review by Assimila: Correction of typos, some links added and some additional explanations given.	All
4.0	18-August-2020	Update for CDR4 (2009-2019)	All
5.0	18-February-2021	Update for CDR5 (2009-mid2020)	All
6.0 Draft	18-February-2022	Update for data set CDR6: First draft	All
6.0	4-August-2022	Update for CDR6: GOSAT-2 retrievals (2019 - 2021)	All
6.1	25-November-2022	Update after review (use of new template, various mostly minor improvements at several places)	All
6.2	31-January-2023	Minor improvements at various places taking into account feedback from 2 <sup>nd</sup> review	All



## List of datasets covered by this document

Deliverable ID	Product title	Product type (CDR, ICDR)	Version number	Delivery date
WP2-FDDP-GHG-v1	CH4_GO2_SRPR	CDR 6	2.0.0	31-Aug-2022

## Related documents

Reference ID	Document
D1	<p>Main ATBD:</p> <p>Buchwitz, M., et al., Algorithm Theoretical Basis Document (ATBD) – Main document for Greenhouse Gas (GHG: CO<sub>2</sub> &amp; CH<sub>4</sub>) data set CDR 6 (2003-2021), project C3S2_312a_Lot2_DLR – Atmosphere, v6.2, 2023.</p> <p><i>(this document is an ANNEX to the Main ATBD)</i></p>
D2	<p>Barr, A. G., et al., Product User Guide and Specification (PUGS) – ANNEX C for product CH4_GO2_SRPR (v2.0.0, 2019-2021), Technical Report C3S project C3S2_312a_Lot2_DLR – Atmosphere, version 6.2, 2023</p>



## Acronyms

Acronym	Definition
AIRS	Atmospheric Infrared Sounder
AMSU	Advanced Microwave Sounding Unit
ATBD	Algorithm Theoretical Basis Document
BESD	Bremen optimal ESTimation DOAS
CAR	Climate Assessment Report
C3S	Copernicus Climate Change Service
CCDAS	Carbon Cycle Data Assimilation System
CCI	Climate Change Initiative
CDR	Climate Data Record
CDS	(Copernicus) Climate Data Store
CMUG	Climate Modelling User Group (of ESA's CCI)
CRG	Climate Research Group
D/B	Data base
DOAS	Differential Optical Absorption Spectroscopy
EC	European Commission
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EMMA	Ensemble Median Algorithm
ENVISAT	Environmental Satellite (of ESA)
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FCDR	Fundamental Climate Data Record
FoM	Figure of Merit
FP	Full Physics retrieval method
FTIR	Fourier Transform InfraRed
FTS	Fourier Transform Spectrometer
GCOS	Global Climate Observing System
GEO	Group on Earth Observation
GEOSS	Global Earth Observation System of Systems
GHG	GreenHouse Gas
GOS	GOSAT
GO2	GOSAT-2
GOME	Global Ozone Monitoring Experiment
GMES	Global Monitoring for Environment and Security
GOSAT	Greenhouse Gases Observing Satellite
GOSAT-2	Greenhouse Gases Observing Satellite 2



IASI	Infrared Atmospheric Sounding Interferometer
IMAP-DOAS (or IMAP)	Iterative Maximum A posteriori DOAS
IPCC	International Panel in Climate Change
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
JAXA	Japan Aerospace Exploration Agency
JCGM	Joint Committee for Guides in Metrology
L1	Level 1
L2	Level 2
L3	Level 3
L4	Level 4
LMD	Laboratoire de Météorologie Dynamique
MACC	Monitoring Atmospheric Composition and Climate, EU GMES project
NA	Not applicable
NASA	National Aeronautics and Space Administration
NetCDF	Network Common Data Format
NDACC	Network for the Detection of Atmospheric Composition Change
NIES	National Institute for Environmental Studies
NIR	Near Infra-Red
NLIS	LMD/CNRS neuronal network mid/upper tropospheric CO <sub>2</sub> and CH <sub>4</sub> retrieval algorithm
NOAA	National Oceanic and Atmospheric Administration
Obs4MIPs	Observations for Climate Model Intercomparisons
OCFP	OCO-2 Full Physics (FP) algorithm (used by Univ. Leicester)
OCO	Orbiting Carbon Observatory
OCPR	OCO-2 Proxy (PR) algorithm (used by Univ. Leicester)
OE	Optimal Estimation
PBL	Planetary Boundary Layer
ppb	Parts per billion
ppm	Parts per million
PQAD	Product Quality Assurance Document
PQAR	Product Quality Assessment Report
PR	(light path) Proxy retrieval method
PVIR	Product Validation and Intercomparison Report
QA	Quality Assurance
QC	Quality Control
RemoTeC	Retrieval algorithm developed by SRON
REQ	Requirement
RMS	Root-Mean-Square
RTM	Radiative transfer model
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY
SCIATRAN	SCIAMACHY radiative transfer model



SRON	SRON Netherlands Institute for Space Research
SRFP	SRON's Full Physics (FP) algorithm (also referred to a RemoTeC FP)
SRPR	SRON's Proxy (PR) algorithm (also referred to a RemoTeC PR)
SWIR	Short Wave Infra-Red
TANSO	Thermal And Near infrared Sensor for carbon Observation
TANSO-FTS	Fourier Transform Spectrometer on GOSAT
TANSO-FTS-2	Fourier Transform Spectrometer on GOSAT-2
TBC	To be confirmed
TBD	To be defined / to be determined
TCCON	Total Carbon Column Observing Network
TIR	Thermal Infra-Red
TR	Target Requirements
TRD	Target Requirements Document
WFM-DOAS (or WFMD)	Weighting Function Modified DOAS
UoL	University of Leicester, United Kingdom
URD	User Requirements Document
WMO	World Meteorological Organization
Y2Y	Year-to-year (bias variability)





## General definitions

### Essential climate variable (ECV)

An ECV is a physical, chemical, or biological variable or a group of linked variables that critically contributes to the characterization of Earth's climate.

### Climate data record (CDR)

The US National Research Council (NRC) defines a CDR as a time series of measurements of sufficient length, consistency, and continuity to determine climate variability and change.

### Fundamental climate data record (FCDR)

A fundamental climate data record (FCDR) is a CDR of calibrated and quality-controlled data designed to allow the generation of homogeneous products that are accurate and stable enough for climate monitoring.

### Thematic climate data record (TCDR)

A thematic climate data record (TCDR) is a long time series of an essential climate variable (ECV).

### Intermediate climate data record (ICDR)

An intermediate climate data record (ICDR) is a TCDR which undergoes regular and consistent updates, for example because it is being generated by a satellite sensor in operation.

### Satellite data processing levels

The NASA Earth Observing System (EOS) distinguishes six processing levels of satellite data, ranging from Level 0 (L0) to Level 4 (L4) as follows.

- L0 Unprocessed instrument data
- L1A Unprocessed instrument data alongside ancillary information
- L1B Data processed to sensor units (geo-located calibrated spectral radiance and solar irradiance)
- L2 Derived geophysical variables (e.g., XCO<sub>2</sub>) over one orbit
- L3 Geophysical variables averaged in time and mapped on a global longitude/latitude horizontal grid
- L4 Model output derived by assimilation of observations, or variables derived from multiple measurements (or both)



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## Scope of the document

This document is an Algorithm Theoretical Basis Document (ATBD) for the Copernicus Climate Change Service (C3S, <https://climate.copernicus.eu/>) greenhouse gas (GHG) component as covered by project C3S2\_312a\_Lot2.

Within this project satellite-derived atmospheric carbon dioxide (CO<sub>2</sub>) and methane (CH<sub>4</sub>) Essential Climate Variable (ECV) data products will be generated and delivered to ECMWF for inclusion into the Copernicus Climate Data Store (CDS) from which users can access these data products and the corresponding documentation.

The GHG satellite-derived data products are:

- Column-averaged dry-air mixing ratios (mole fractions) of CO<sub>2</sub> and CH<sub>4</sub>, denoted XCO<sub>2</sub> (in parts per million, ppm) and XCH<sub>4</sub> (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO<sub>2</sub> (in ppm) and CH<sub>4</sub> (in ppb).

This document describes the retrieval algorithm used to generate the C3S product CH<sub>4</sub>\_GO<sub>2</sub>\_SRPR v2.0.0.

This product is the XCH<sub>4</sub> Level 2 product as retrieved from GOSAT-2 using algorithms developed at SRON, The Netherlands.



## Executive summary

In this document the retrieval algorithms are described, which are used to generate satellite-derived atmospheric carbon dioxide (CO<sub>2</sub>) and methane (CH<sub>4</sub>) Climate Data Record (CDR) data products as generated via the C3S2\_312a\_Lot2 project of the Copernicus Climate Change Service (C3S, <https://climate.copernicus.eu/>).

This document describes the RemoTeC algorithm for GHG retrieval from the GOSAT-2 instrument. It should be read in conjunction with the MAIN ATBD document, defined in the Related Documents section at the beginning of this document (D2). The original algorithm is based on the paper of Butz et al., 2009. Tests of the retrieval algorithm have been performed on synthetic GOSAT data (Butz et al., 2010), and real GOSAT data (Butz et al., 2011; Schepers et al., 2012; Guerlet et al., 2012). Here we apply the retrieval to GOSAT-2 data.

The RemoteC algorithm developed by SRON is a linearized vector radiative transfer model which solves the equation of radiative transfer for back-scattered sunlight. It adopts Philips-Tikonov regularization to apply the inversion, and the Gauss-Sidel method to solve the equation of radiative transfer. The retrieval algorithm aims at inferring an atmospheric state vector from a measurement vector. The state vector is linked to the measurement vector through the true forward model.

In order to account for the effect of aerosols and cirrus, the proxy method retrieves both the CH<sub>4</sub> and CO<sub>2</sub> column under the assumption of a non-scattering atmosphere assuming that scattering effects cancel by taking the ratio of the 2 is calculated. XCH<sub>4</sub> is then calculated by multiplying the ratio with XCO<sub>2</sub> obtained from a model (CarbonTracker 2013 or LMD CO<sub>2</sub> flask inversions). Additional fit parameters are the surface albedo and its 1st order spectral dependence in all bands, and the total column of water vapor, respectively.

In order to obtain a proper characterization of the retrieved XCH<sub>4</sub>, it is important to first retrieve a vertical profile (layer averaged number density in different layers of the model atmosphere) and use this retrieved vertical profile to calculate the vertical column. Here, we choose to provide the vertical column as a product, and not the full profile, because the Degrees of Freedom for Signal (DFS) of the retrieved CH<sub>4</sub> and CO<sub>2</sub> profile is about 1. The inversion is performed using Phillips-Tikhonov regularization in combination with a reduced step size Gauss-Newton iteration scheme.

The greenhouse gas (GHG) activities of this C3S project and its C3S pre-cursor projects are essentially the operational continuation of the research and development (R&D) pre-cursor projects GHG-CCI and GHG-CCI+ of ESA's Climate Change Initiative (CCI). R&D for the GOSAT-2 products is currently an ongoing activity of the ESA GHG-CCI+ project (see <https://climate.esa.int/en/projects/ghgs/>).

Section 1 gives an overview of the data product including a description of the GOSAT-2 satellite. Section 2 introduces the various input data which enter into the retrieval algorithm such as



meteorological data, satellite level 1 data and a priori CH<sub>4</sub>/CO<sub>2</sub> profiles. Sections 3 and 4 describe in detail the retrieval algorithm and its output, respectively.



## 1. Instruments

In this section an overview of the data product (specified in terms of variable, its property, processing level(s) and instrument(s)) are given. In the following, two satellite instruments are briefly described which are used / can be used to generate the XCH<sub>4</sub> data product CH<sub>4</sub>\_GO2\_SRPR.

### 1.1 TANSO-FTS-2 on GOSAT-2

The Japanese Greenhouse gases Observing SATellite-2 (GOSAT-2) was launched on 29th October 2018 and started operational observations from February 2019. GOSAT-2 provides dedicated global measurements of total column CO<sub>2</sub> and CH<sub>4</sub> from its Short Wave Infra-red (SWIR) bands. It is equipped with two instruments, the Thermal And Near Infrared Sensor for carbon Observations - Fourier Transform Spectrometer-2 (TANSO-FTS2) as well as a dedicated Cloud and Aerosol Imager-2 (TANSO-CAI-2).

The TANSO-FTS2 instrument (Nakajima et al., 2017) has five spectral bands, given in Table 1, with a high spectral resolution 0.2 cm<sup>-1</sup>. Three operate in the SWIR at 0.75-0.77, 1.56-1.69 and at the extended 1.92-2.33 μm range, providing sensitivity to the near-surface absorbers. The fourth and fifth channels operating in the thermal infrared between 5.5-8.4 and 8.4-14.3 μm providing mid-tropospheric sensitivity.

FTS-2 observes sunlight reflected from the earth's surface and light emitted from the atmosphere and the surface. The former is observed in the spectral bands 1 through 3 of FTS in the daytime, and the latter is captured in band 4 and 5 during both the day and the night. Within this project only level 1 data from the SWIR channels 1-3 will be used. Prior to reaching the detectors of the instrument, the light in the bands 1 through 3 is split into two orthogonally-polarized components and measured independently. The intensity component of Stokes vector is approximated by the mean of parallel (P) and perpendicular (S) components (O'Brien et al., 2013).

The measurement strategy of TANSO-FTS-2 is optimized for the characterization of continental-scale sources and sinks. TANSO-FTS-2 utilizes a pointing mirror to perform off-nadir measurements at the same location on each 6-day repeat cycle. The pointing mirror allows TANSO-FTS-2 to observe up to ±35° across track and ±40° along-track. These measurements nominally consist of 5 across track points spaced ~160km apart with a ground footprint diameter of approximately 9.7 km and a 4 second exposure duration. The satellite has an Intelligent pointing Monitor camera which makes it possible to adjust the line of sight of the FTS to steer away from cloud contaminated areas. Whilst the majority of data is limited to measurements over land where the surface reflectance is high, TANSO-FTS-2 also observes in sunglint mode over the ocean. More information on GOSAT-2 can be found here: <http://www.gosat-2.nies.go.jp/>.



Table 1: GOSAT-2-FTS bands

Channel	Wavelength range [nm]	Resolution [ $\text{cm}^{-1}$ ]
1	758-775	0.2
2	1460-1720	0.2
3	1920-2330*	0.2
4	5560-8400	0.2
5	8400-14300	0.2

\*GOSAT-1 only had a spectral range up to 2080nm.



## 2. Input and auxiliary data

TANSO-FTS-2 level-1b data are available since February 2019. The GOSAT-2 FTS L1A/L1B Product Description Document (Japan Aerospace Exploration Agency, July 2019, GST-18005) is available through [https://prdct.gosat-2.nies.go.jp/documents/pdf/NIES\\_GOSAT-2\\_Product\\_File\\_Format\\_Descriptions\\_en\\_03.pdf](https://prdct.gosat-2.nies.go.jp/documents/pdf/NIES_GOSAT-2_Product_File_Format_Descriptions_en_03.pdf)

The quality of the retrieved CO<sub>2</sub> and CH<sub>4</sub> columns has been tested against ground-based observations, i.e. the TCCON network (Wunch 2011, 2015), and has shown to be of good quality. The spectral bands showed some irregularities which required a shortened retrieval window (O<sub>2</sub> A-band) and spectral intensity offsets for each of the bands. This in effect worsened the cost function  $\chi^2$  of the fits compared to similar GOSAT-1 retrievals and the estimated uncertainties of the species. However, comparison to TCCON observations showed that the retrieval products of both the GOSAT-1 and GOSAT-2 are of similar quality.

### 2.1 Other data

#### 2.1.1 ECMWF model data

The retrieval algorithms to produce vertical columns of CO<sub>2</sub> and CH<sub>4</sub> need as input for each scene the temperature vertical profile, pressure vertical profile, specific humidity vertical profile, and wind speed. Here, temperature and pressure are needed to calculate absorption cross sections, the specific humidity vertical profile is needed to account for water vapor absorption, and the wind speed is needed to calculate the Fresnel reflection contribution on a rough ocean surface. The meteorological data mentioned above will be taken from the ECMWF model.

*Originating system:* ECMWF has developed one of the most comprehensive earth-system models available anywhere. The ECMWF model uses the '4D-Var' data assimilation approach, which provides a physically consistent best fit to observations. For this project the ERA-5 data are used.

*Data class:* Model

*Required ECMWF data:*

*Class:* ERA-5

*Stream:* Atmospheric model

*Type:* Analysis

*Dates:* 01/08/2019 to present

*Time:* 00:00:00, 03:00:00, 06:00:00, 09:00:00, 12:00:00, 15:00:00, 18:00:00, 21:00:00

*Spatial grid:* T639 Quasi-uniform Gaussian grid (~0.28°, 31km)





Parameters at model levels:

- temperature, specific humidity (all levels)
- logarithm of surface pressure, geopotential (lowest level)

Parameters at surface:

- 10 meter U wind component
- 10 meter V wind component

*Data availability & coverage:* All data are required on a global scale, with a typical delay of three months.

*Data quality and reliability:* The ECMWF model data sets are widely considered to be among the best available data sets for meteorological parameters. We have compared retrievals for an overlapping month (August 2019) using both ERA-5 and ERA-interim and no major effects were observed in the retrieved parameters.

### 2.1.2 Carbon Tracker Data

The retrieval algorithms for CH<sub>4</sub> columns from SCIAMACHY, GOSAT, and GOSAT-2 that are based on the "proxy approach" retrieve the ratio of the CH<sub>4</sub> and CO<sub>2</sub> columns, where the CO<sub>2</sub> column serves as a proxy for the light path. In order to obtain the CH<sub>4</sub> column, the retrieved ratio needs to be multiplied by the best estimate of the CO<sub>2</sub> column. It is assumed that data from the Carbon Tracker model can provide the best estimate of the true CO<sub>2</sub> column.

*Originating system:*

Carbon Tracker is a data assimilation system developed at the National Oceanic and Atmospheric Administration's (NOAA's) Earth System Research Laboratory (ESRL). It is based on a state-of-the-art atmospheric transport model coupled to an ensemble Kalman filter. CarbonTracker assimilates atmospheric CO<sub>2</sub> mole fractions, using a variety of in situ measurements worldwide.

*Data class:* Model

*Data availability & coverage:*

CarbonTracker provides global daily data at a spatial resolution of 3 by 2 degree. Data are available with a delay typically of one or more years.

*Source data product name & reference to product technical specification documents*

CarbonTracker 3D Mole Fractions

Peters, W. et al. (2007)

*Data quality and reliability*

CarbonTracker has been validated with many independent measurements and is considered to provide be an accurate global CO<sub>2</sub> data set.



### 2.1.3 CO<sub>2</sub> correction data

In order to obtain the CH<sub>4</sub> column, the retrieved ratio needs to be multiplied by the best estimate of the CO<sub>2</sub> column. Instead of using CO<sub>2</sub> column values from CarbonTracker, we can use the data from the LMD CO<sub>2</sub> flask inversions as alternative choice. It is assumed that data from the LMD flask inversion can provide the best up-to-date estimate of the true CO<sub>2</sub> column.

*Originating system:*

The inversion product used here is the official CAMS v18r1 product that assimilates about 130 sites of surface air sample measurements from the Global Atmosphere Watch programme

*Data class: Model*

*Data availability & coverage:*

The CAMS v18r1 inversion product provides global 3-hourly data at a spatial resolution of 3.75 by 1.89 degree. Data are typically available within one year.

*Source data product name & reference to product technical specification documents*

*Chevalier et al 2010.*

*Data quality and reliability*

The CAMS v16r1 inversion product has been validated with many independent measurements and is considered to provide be an accurate global CO<sub>2</sub> data set. For the year 2019, we use the CAMS v18r1 product for the year 2018 by taking into account an annual increase of 2.75 ppm.

### 2.1.4 SRTM DEM

The RemoTeC retrieval algorithm for CO<sub>2</sub> and CH<sub>4</sub> columns from GOSAT-2 use information about the surface elevation from an extended SRTM digital elevation map.

*Originating system:* The original Shuttle Radar Telemetry Mission (SRTM) was provided by the United States National Aeronautics and Space Administration (NASA). The dataset used (DEM3) is based on the SRTM dataset and includes extrapolation and gap filling from various sources.

*Data class: Model*

*Sensor type and key technical characteristics:*

n/a

*Data availability & coverage:*

The original SRTM dataset provides elevation data ranging from 56 degrees south to 60 degrees north at a 90 meter resolution. The adjusted DEM3 dataset extends the coverage, while keeping the 90 meter resolution.



*Source data product name & reference to product technical specification documents:*

<http://www.viewfinderpanoramas.org/dem3.html>

### 2.1.5 TCCON FTS CO<sub>2</sub> and CH<sub>4</sub> data

TCCON data for CO<sub>2</sub> and CH<sub>4</sub> is available for public for all TCCON stations (<https://tccon-wiki.caltech.edu/>). We use the GGG2014 official release of the data product.

*Originating system:* Ground based

*Data class:* Ground based

*Sensor type and key technical characteristics:*

The measurements are performed using the solar absorption spectroscopy in the near infrared using a Fourier Transform Spectrometer (FTS).

*Data availability & coverage:*

Coverage is limited to the locations of the TCCON stations themselves. Depending on the instrument setting (gain H, gain M or sunlint), we use different TCCON stations for validation (see Product User Guide). Data is typically available only after one year, although some stations deliver on a more regular interval (3 months).

*Source data product name & reference to product technical specification documents:*

*Wunch et al., 2011*

*Data quantity:*

Individual measurements can be taken in intervals of about 20 min. The observations can only be taken with the direct sunlight. This limits the amount of data, which is different from site to site.

*Data quality and reliability:*

For XCO<sub>2</sub> the precision is 0.25% (1ppm) and the systematic error (bias) is 0.2% (0.8 ppm). For XCH<sub>4</sub> the precision is 0.40% (7ppb) and the systematic error (bias) is also 0.40% (7 ppb).



### 2.1.6 TANSO-FTS on GOSAT

The precursor of the TANSO-FTS2 is the TANSO-FTS onboard the Japanese GOSAT satellite (Kuze et al., 2009, 2014, 2016). The Greenhouse Gases Observing Satellite "IBUKI" (GOSAT) is the world's first spacecraft in orbit dedicated to measure the concentrations of carbon dioxide and methane from space. The spacecraft was launched successfully on January 23, 2009, and has been operating properly since then. GOSAT covers the relevant CO<sub>2</sub>, CH<sub>4</sub> and O<sub>2</sub> absorption bands in the NIR and SWIR spectral region as needed for accurate XCO<sub>2</sub> and XCH<sub>4</sub> retrieval (in addition GOSAT also covers a large part of the Thermal Infrared (TIR) spectral region). The spectral resolution of TANSO-FTS is 0.24 to 0.367 cm<sup>-1</sup> and the ground pixels are 10 km with a circular footprint. The GOSAT scan pattern consists of non-consecutive individual ground pixels, i.e., the scan pattern is not gap-free. For a good general overview about GOSAT see also <http://www.gosat.nies.go.jp/en/>.

### 2.1.7 Additional input data

- Absorption cross sections: For the retrieval lookup-tables are used with pre-calculated absorption cross sections of the species of interest (O<sub>2</sub>, CO<sub>2</sub>, CH<sub>4</sub>, and H<sub>2</sub>O) as a function of wavenumber, temperature, and pressure. One lookup-table per species and per spectral band is being used.
- Aerosol optical properties: A lookup table is being used with pre-calculated aerosol optical properties (Mie and t-Matrix theory) as a function of size parameter and refractive index.
- Solar source: The solar source for the forward simulation uses data of extraterrestrial irradiance from the Total and Spectral Solar Irradiance Sensor-1 Hybrid Solar Reference Spectrum (TSIS-1 HSRS). It covers a temporally constant irradiance spectrum between 200 and 2700 nm with a spectral resolution of 0.001 nm (Coddington et al., 2021). The TSIS-1 HSRS data is downloaded from [https://lasp.colorado.edu/lisird/data/tsis1\\_hsr](https://lasp.colorado.edu/lisird/data/tsis1_hsr).
- Retrieval settings: A file is read in with retrieval settings such as spectral range and 5 other parameters.



### 3. Algorithms

#### 3.1 Algorithm description

Any retrieval algorithm aims at inferring an atmospheric state *vector*  $x$  from a measurement vector  $y$ . The state vector is linked to the measurement vector through the true forward model  $f(x,b)$  that depends on the state *vector*  $x$  and the *vector*  $b$  containing ancillary parameters that are not retrieved,

$$y = f(x, b) + e_y \quad (1)$$

Where  $e_y$  represents the measurement noise vector. A retrieval method approximates the true forward model  $f$  by a retrieval forward model  $F$ , with a forward model error vector  $e_F$ ,

$$y = F(x, b) + e_y + e_F \quad (2)$$

For full physics retrieval from the GOSAT-2 FTS instrument the measurement vector contains the measured intensities in the NIR and SWIR (see Table 2).

Table 2: Spectral ranges from the NIR and SWIR band included in the measurement vector

Band	Used spectral range
1 (O <sub>2</sub> a)	12950 – 13195 cm <sup>-1</sup>
2 (CO <sub>2</sub> )	6170 – 6277 cm <sup>-1</sup>
3 (CH <sub>4</sub> )	6045 – 6138 cm <sup>-1</sup>
4 (CO <sub>2</sub> )	4806 – 4896 cm <sup>-1</sup>

For the retrieval procedure it is needed that the non-linear forward model is linearised so that the retrieval problem can be solved iteratively. For iteration step  $n$  the forward model is approximated by

$$F(x, b) \approx F(x_n, b) + K(x_n - x) \quad (3)$$

Where  $x_n$  is the state vector for the  $n$ -th iteration step and  $K$  is the Jacobian matrix

$$K = \frac{\partial F}{\partial x} \quad (4)$$



Below, we will describe the retrieval forward model, state vector, ancillary parameter vector, and the inversion method in more detail.

### 3.2 Forward Model

The retrieval forward model  $F$  simulates the measurement vector  $y$  for a given model atmosphere defined by the state vector  $x$  and the ancillary parameter vector  $b$ . The simulated intensity for a given spectral pixel  $i$  is given by

$$I_i = \int_{\lambda_{min}}^{\lambda_{max}} I(\lambda) S_i(\lambda) d\lambda \quad (5)$$

Where  $S_i(\lambda)$  is the Instrument Spectral Response Function (ISRF) for spectral pixel  $i$  and  $I(\lambda)$  is the modeled intensity at high spectral resolution. In the NIR and SWIR channel  $I(\lambda)$  contains many fine spectral structures due to molecular absorption, so it has to be calculated at fine spectral resolution (0.1 cm<sup>-1</sup> in the NIR band and 0.02 cm<sup>-1</sup> in the SWIR).

#### 3.2.1 Model Atmosphere and Optical Properties

For the RemoTeC algorithm described here the model atmosphere is defined for  $NLAY=36$  homogeneous vertical layers that are equidistant in pressure, the lowest pressure level being defined by the surface pressure. The absorbing trace gases of interest are O<sub>2</sub> (in the NIR band) and CH<sub>4</sub>, H<sub>2</sub>O, and CO in the SWIR band. The layer sub-columns of these gases are for the first iteration step of each retrieval calculated from the input profiles of CH<sub>4</sub>, CO (TM5) and H<sub>2</sub>O (ECMWF) and the temperature and pressure profiles (ECMWF). They are obtained on the grid of the model atmosphere by linear interpolation. Here, first the surface pressure  $p_{surf}$  is obtained by interpolation of the input pressure profile as function of height to the surface height (input) for the corresponding ground pixel. Next the pressure values at the layer boundaries are calculated, with the pressure  $p_k$  at the lower boundary of layer  $k$  (counting from top to bottom) is given by:

$$p_{lev,k} = p_{min} + \Delta p * k \quad (6)$$

Where:

$$\Delta p = \frac{p_{surf} - p_{min}}{NLAY} \quad (7)$$

Where  $p_{min}$  is the pressure value of the upper boundary of the input (ECMWF) atmosphere. The different atmospheric profiles are constructed on this pressure grid. For example, the methane sub-column  $DV\_CH4_k$  for the layer bounded by pressure levels  $p_{lev,k}$  and  $p_{lev,k+1}$  is given by:



$$DV\_CH4_k = XCH4_k \times DV\_AIR_k \quad (8)$$

Where  $XCH4_k$  is the methane dry air mixing ratio linearly interpolated from the input pressure grid to the pressure at the 'middle' of layer  $k$  defined by  $(p_k + p_{k+1})/2$ .  $DV\_AIR_k$  is the sub-column of air in layer  $k$ , given by

$$DV\_AIR_k = (p_{lev,k+1} - p_{lev,k}) \times R / (M \times g_k \times \left(1 + \frac{XH_2O_k}{1.60855}\right)) \quad (9)$$

Where  $R$  is Avogadro's number,  $M$  is the molecular mass of air,  $g_k$  is the gravity constant in altitude layer  $k$ , and 1.60855 is the mass of air relative to the mass of water (Wunch et al., 2010). The sub-columns of CO and H<sub>2</sub>O are calculated in the same manner as for CH<sub>4</sub>, and the O<sub>2</sub> sub-column is obtained by multiplying the air sub-column by the O<sub>2</sub> mixing ratio (=0.2095).

In the proxy method scattering is neglected in the forward model and hence atmospheric scattering properties do not need to be calculated.

To summarize, the forward model needs the following inputs:

- Surface pressure to define the equidistant pressure grid
- Sub-columns of CH<sub>4</sub>, CO, H<sub>2</sub>O, O<sub>2</sub>, and air for the vertical layers of the model atmosphere.
- Pressure and temperature at the middle of the model sub-layers for absorption cross-sections.
- Solar Zenith Angle (SZA).
- Viewing Zenith Angle (VZA).
- Relative Azimuth Angle (RAA).
- The aerosol complex refractive index  $m = m_r + im_i$
- A high spectral resolution solar reference spectrum.
- Lookup tables with absorption cross-sections of CH<sub>4</sub>, CO, H<sub>2</sub>O, and O<sub>2</sub> as function of pressure, temperature, and wavenumber.

Based on these inputs the optical properties can be calculated for each layer of the model atmosphere.



### 3.2.2 Modeling the top-of-atmosphere radiances

For the proxy method the top of the atmosphere radiance can be modeled using the Lambert Beers law and surface reflection:

$$I_{TOA} = R_{surf} F_0 e^{-\left(\frac{\tau}{\mu_0} + \frac{\tau}{\mu_v}\right)} \quad (10)$$

where  $F_0$  is the incoming total flux,  $\tau = \tau_{abs}$ ,  $\mu_0$  is the cosine of the solar zenith angle,  $\mu_v$  is the cosine of the viewing zenith angle, and  $R_{surf}$  is the surface reflection for the specific solar and viewing geometry under consideration.

### 3.3 Inverse algorithm

*Definition of state vector and ancillary parameters*

The **state vector**  $\mathbf{x}$  contains the following elements listed in Table 3 (between brackets are optional elements):

- CO<sub>2</sub> sub-columns in 12 vertical layers (layer interfaces coincide with  $NLAY$  layers of forward model grid).
- CH<sub>4</sub> sub-columns in 12 vertical layers (layer interfaces coincide with  $NLAY$  layers of forward model grid).
- H<sub>2</sub>O total column.
- Lambertian surface albedo in all bands band.
- First order spectral dependence of surface albedo in all bands.
- Spectral shift of Earth radiances in all bands (higher orders optional).
- Spectral shift of Earth radiances in all bands (higher orders optional).
- (offset in input temperature profile).
- (surface pressure).

For convergence it was essential to include intensity offsets to each of the individual spectral windows. Potentially there are still irregularities in the quality of the individual spectral bands.

The **ancillary parameter vector**  $\mathbf{b}$  contains the following parameters:

- H<sub>2</sub>O sub-columns in 36 vertical layers of forward model grid.
- Temperature vertical profile at 72 layers of cross-section vertical grid.
- Pressure vertical profile at 72 layers of cross-section vertical grid.





Table 3: A priori values for the different state vector elements.

State vector element	A priori value
CH <sub>4</sub> sub-columns	TM4
CO <sub>2</sub> sub-columns	Carbontracker
H <sub>2</sub> O total column	ECMWF
surface albedo (NIR + SWIR)	no prior value needed (first guess at maximum of measured reflectance)
spectral shifts	no prior needed (first guess = 0)
temperature offset	no prior needed (first guess = 0)
surface pressure	ECMWF + SRTM DEM

### 3.3.1 Inversion Procedure

The inverse method optimizes the state vector  $x$  with respect to the measurements  $y$  after applying the forward model  $F$  to  $x$ . The inverse method is based by default on a Phillips-Tikhonov regularization scheme (Phillips, 1962; Tikhonov, 1963; Hasekamp and Landgraf, 2005). Regularization is required because the inverse problem is ill-posed, i.e., the measurements  $y$  typically contain insufficient information to retrieve all state vector elements independently. The inverse algorithm finds  $x$  by minimizing the cost function that is the sum of the least-squares cost function and a side constraint weighted by the regularization parameter  $\gamma$  according to

$$\hat{x} = \min_x ( \|S_y^{-\frac{1}{2}}(F(x) - y)\|^2 + \gamma \|W(x - x_a)\|^2 ) \quad (11)$$

Where  $S_y$  is the diagonal measurement error covariance matrix, which contains the noise estimate.  $x_a$  is an a priori state vector (see Table 3), and  $W$  is a weighting matrix (see below).

For the linearised forward model for iteration step  $n$ , the equation for the updated state vector  $x_{n+1}$  reduces to

$$x_{n+1} = \min ( \|K'(x' - x'_n - y')\|^2 + \gamma \|x' - x'_n\|^2 ) \quad (12)$$

With the weighted quantities

$$x' = Wx, \quad y' = S_y^{-\frac{1}{2}}(y - F(x_n)) \quad (13)$$



and

$$K' = S_y^{-1/2} K W^{-1} \quad (14)$$

The solution reads

$$x_{n+1} = G' y' + A' x'_n + (I - A') x'_{apr} \quad (15)$$

With  $A'$  the averaging kernel matrix and  $G'$  the contribution function matrix given by

$$A' = G' K' \quad (16)$$

and

$$G' = (K'^T K' + \gamma I)^{-1} K'^T \quad (17)$$

If the retrieval converges after a given number of steps  $N$  (typically 7-8), the final state vector  $x_{retr} = x_N$  is related to the true state vector and to the prior via

$$x_{retr} = A x_{true} + (I - A) x_n + G e_y + G e_F \quad (18)$$

The covariance matrix  $S_x$  describing the retrieval noise ( $G e_y$ ) is given by

$$S_x = G S_y G^T \quad (19)$$

The target retrieval quantity is the column averaged dry air  $\text{CH}_4$  mixing ratio,  $X\text{CH}_4$ . This quantity is obtained from the  $\text{CH}_4$  and  $\text{CO}_2$  entries of the retrieved state vector through

$$X\text{CH}_4 = \frac{V_{ch4}}{V_{co2}} \times X\text{CO}_{2,prior} \quad (20)$$

where  $V_{ch4}$  and  $V_{co2}$  are the total columns of  $\text{CO}_2$  and  $\text{CH}_4$ , respectively, obtained from the retrieval state vector by

$$V_{ghg} = h_{ghg}^T x_{retr} \quad (21)$$

where the subscript  $ghg$  refers to either  $\text{CO}_2$  or  $\text{CH}_4$ ,  $h$  is the total column operator (summing up the partial columns in the state vector). The retrieval noise  $\Delta X\text{CH}_4$  on  $X\text{CH}_4$  is given by





parameters, and 0 for all other parameters (which means they are not constrained by the side constraint and are retrieved in a least-squares sense). The value for  $\gamma$  is fixed such that the Degrees of Freedom for Signal (DFS) for the methane profile is in the range 1.0-1.5. This value is found empirically.

### 3.4 Cloud Filtering

Cloud filtering in RemoTeC proxy is based on retrieved columns of oxygen ( $VO_2$ ), carbon dioxide ( $VCO_2$ ) and water vapor ( $VH_2O$ ) retrieved independently from the 0.75 micron, 1.6 micron, and 2.0 micron bands, respectively, under the assumption of a non-scattering atmosphere:

$0.88 < VO_2\_retrieved / VO_2\_ecmwf < 1.035$ ,  $0.98 < VCO_2\_1.6micron / VCO_2\_2.0micron < 1.15$ ,  
 $0.90 < VH_2O\_1.6micron / VH_2O\_2.0micron < 1.5$ . The rationale for these cloud filters is that scenes with a large light path deviation with respect to a non-scattering atmosphere will result in different  $CO_2$  and  $H_2O$  columns retrieved (without scattering) from the 1.6 and 2.0 micron band due to different light path sensitivities in the two bands. Also, the retrieved  $O_2$  column will deviate more from the ECMWF  $O_2$  column for large light path differences with a non-scattering atmosphere. For the proxy the cloud filters are less strict than for the Full Physics Algorithm as the ratio retrieved in the proxy method is less sensitive to cloud contamination.



## 4. Output data

The output data are stored in one NetCDF file per day. The file size varies between 1 and 5 Mb.

The files are named as follows:

ESACCI-GHG-L2-CH4-GOSAT2-SRFP-YYYYMMDD-fv1.nc

Where YYYY, MM and DD denote the year, month and day respectively. The formatting of the files is in accordance with CF-1.6 convention standards and the variables names correspond to CF Standard Name Table v79. There is a quality flag “xch4\_quality\_flag” included in the data files. The quality flag can have 2 values:

- 0: retrieval quality has been checked
- 1: data should not be used (e.g. bad fit to data, residual cloud contamination)

Pixels flagged with 1 include those pixels rejected by post-processing quality filtering steps. After the retrieval step the data that fulfill the following criteria are flagged as '0' for land and '1' for ocean (glint).

An important step in the post-processing is the bias correction (see the Product User Guide and Specification (PUGS) [D2] for details). As a result, two variables are provided for CH<sub>4</sub>, defined as xch4 and raw\_xch4 for the bias corrected and non-bias corrected columns, respectively.

Note that the format of the main output data, which are the Level 2 data products, is described in the associated Product User Guide and Specification (PUGS) document (document D2 defined in the Related Documents at the start of this document).



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