ECMWF COPERNICUS REPORT

Copernicus Climate Change Service

Algorithm Theoretical Basis Document (ATBD) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR6 (01.2003-12.2021)

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 (temporal coverage: 2003-2016)	All
2.0	16-October-2018	Update for data set CDR2 (temporal coverage: 2003-2017)	All
3.0	12-August-2019	Update for data set CDR3 (temporal coverage: 2003-2018)	All
3.1	03-November-2019	Update after review: Correction of typos and broken links	All
4.0	18-August-2020	Update for data set CDR4 (temporal coverage: 2003-2019)	All
5.0	17-February-2021	Update for data set CDR5 (temporal coverage: 01.2003-06.2020)	All
6.0 Initial Draft	18-February-2022	Initial draft for data set CDR6	All
6.0	4-August-2022	Update for data set CDR6 (temporal coverage: 01.2003-12.2021)	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 2nd 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	CO2_GOS_OCFP (ANNEX A)	CDR 6	7.3	31-Aug-2022
WP2-FDDP-GHG-v1	CH4_GOS_OCFP (ANNEX A)	CDR 6	7.3	31-Aug-2022
WP2-FDDP-GHG-v1	CH4_GOS_OCPR (ANNEX A)	CDR 6	9.0	31-Aug-2022
WP2-FDDP-GHG-v1	CO2_GO2_SRFP (ANNEX B)	CDR 6	2.0.0	31-Aug-2022
WP2-FDDP-GHG-v1	CH4_GO2_SRFP (ANNEX B)	CDR 6	2.0.0	31-Aug-2022
WP2-FDDP-GHG-v1	CH4_GO2_SRPR (ANNEX C)	CDR 6	2.0.0	31-Aug-2022
WP2-FDDP-GHG-v1	XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, XCH4_OBS4MIPS (ANNEX D)	CDR 6	4.4	31-Aug-2022
WP2-FDDP-GHG-v1	CO2_IASA_NLIS, CH4_IASA_NLIS, CO2_IASB_NLIS, CH4_IASB_NLIS (ANNEX E)	CDR 6	9.1	31-Aug-2022

(*) In brackets: see listed ANNEX to this MAIN document for details on listed product(s).

Related documents

Reference ID	Document
D1	**GCOS-154:** Global Climate Observing System (GCOS): SYSTEMATIC OBSERVATION REQUIREMENTS FOR SATELLITE-BASED DATA PRODUCTS FOR CLIMATE - 2011 Update - Supplemental details to the satellite-based component of the "Implementation Plan for the Global Observing System for Climate in Support of the UNFCCC (2010 Update)", December 2011, prepared by World Meteorological Organization (WMO), Intergovernmental Oceanographic Commission, United Nations Environment Programme (UNEP), International Council for Science, Doc.: GCOS 154, link: http://cci.esa.int/sites/default/files/gcos-154.pdf, 2011.
D2	**GCOS-200:** The Global Observing System for Climate: Implementation Needs, World Meteorological Organization (WMO), GCOS-200 (GOOS-214), pp. 325, link: http://unfccc.int/files/science/workstreams/systematic_observation/application/pdf/gcos_ip_10oct2016.pdf, 2016.
D3	**ESA-CCI-GHG-URDv2.1:** Chevallier, F., et al., User Requirements Document (URD), ESA Climate Change Initiative (CCI) GHG-CCI project, Version 2.1, 19 Oct 2016, https://www.iup.uni-bremen.de/carbon_ghg/docs/GHG-CCIplus/URD/URDv2.1_GHG-CCI_Final.pdf, 2016.
D4	**TRD GAD GHG, 2021:** Buchwitz, M., Reuter, M., Schneising-Weigel, O., Aben, I., Wu, L., Hasekamp, O. P., Boesch, H., Di Noia, A., Crevoisier, C., Armante, R.: Target Requirement and Gap Analysis Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO_2 and CH_4) data products, Version 3.1, 19-February-2021, pp. 81, 2021. Latest version: http://wdc.dlr.de/C3S_312b_Lot2/Documentation/GHG/C3S2_312a_Lot2_TRD-GAD_GHG_latest.pdf
D5	**PUGS GHG, 2023:** Buchwitz, M., Barr, A., Boesch, H., Borsdorff, T., Crevoisier, C., Di Noia, A., Hasekamp, O. P., Landgraf, J., Meilhac, N., Parker, R., Reuter, M., Schneising-Weigel, O.: Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO_2 & CH_4) data set CDR6 (01.2003-12.2021), C3S project C3S2_312a_Lot2_DLR, v6.2, 2023

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 CO2 and CH4 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 Wava 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 (Bojinski et al., 2014).

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 (National Research Council, 2004).

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) (Werscheck, 2015).

Intermediate climate data record (ICDR)

An intermediate climate data record (ICDR) is a TCDR which undergoes regular and consistent updates (Werscheck, 2015), 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 (Parkinson et al., 2006).

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_2) 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)

The C3S GHG data products include the following types of data:

Level 2 data:

- Individual sensor and multi-sensor merged CO_2 and CH_4 retrievals for each (quality flagged) satellite ground-pixel

Level 3 data:

- Gridded monthly averages (5° x 5°) covering the globe in Obs4MIPs format

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Scope of the document

This document is the Algorithm Theoretical Basis Document (ATBD) for the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) component as covered by the greenhouse gas (GHG) activities of project C3S2_312a_Lot2 led by DLR, Germany (the follow-on project of projects C3S_312b_Lot2, led by DLR, and project C3S_312a_Lot6, led by University of Bremen, Germany), in the following referred to as C3S/GHG project or simply as project.

Within this C3S/GHG project, satellite-derived atmospheric carbon dioxide (CO_2) and methane (CH_4) Essential Climate Variable (ECV) data products have been generated and provided to ECMWF for inclusion into the Copernicus Climate Data Store (CDS) from which users can access these data products and the corresponding documentation.

The C3S/GHG satellite-derived data products are:

- Column-averaged dry-air mixing ratios (mole fractions) of CO_2 and CH_4, denoted XCO_2 (in parts per million, ppm) and XCH_4 (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO_2 (in ppm) and CH_4 (in ppb).

An overview about the products is given in Table 1 for the CO_2 products and in Table 2 for the CH_4 products.

Requirements on data quality are formulated in the corresponding Target Requirement Document (TRD) (*D4*).

The main purpose of this document is to describe the retrieval algorithms, which are used to generate the satellite-derived CO_2 and CH_4 greenhouse gas (GHG) ECV data products. Specifically, this document is the main ATBD providing “only” an overview of all products and their underlying retrieval algorithms. Details on each algorithm, or group of similar algorithms, are described in a set of Annexes to this document (see Sect. 6 List of ANNEXES).

For an overview of the merged Level 2 data products XCO2_EMMA and XCH4_EMMA and of the merged Level 3 data products XCO2_OBS4MIPS and XCH4_OBS4MIPS see also Reuter et al., 2020.

Table 1: Overview CO_2 products. "CRD#" indicates the Climate Data Record (CDR) Number. Level 2 (L2) products contains information for each individual satellite footprint (ground pixel) whereas Level 3 (L3) products are gridded /averaged spatially and temporally.

Product ID (Level)	Version	CDR#	Temporal coverage	Comments
CO2_GOS_OCFP (L2)	7.3	4-6	04.2009 – 12.2021	XCO_2 from GOSAT as retrieved with Univ. Leicester's OCFP algorithm.
CO2_GO2_SRFP (L2)	2.0.0	6	02.2019 – 12.2021	XCO_2 from GOSAT-2 as retrieved with SRON's SRFP (RemoTeC) algorithm.
XCO2_EMMA (L2)	4.4	6	01.2003 – 12.2021	Merged L2 XCO_2 product using Univ. Bremen's EMMA algorithm.
XCO2_OBS4MIPS (L3)	4.4	6	01.2003 – 12.2021	Merged L3 XCO_2 product in OBS4MIPS format.
CO2_IASA_NLIS (L2)	9.1	4-6	07.2007 – 08.2021	Mid-tropospheric CO_2 mixing ratios as retrieved from IASI/Metop-A using LMD's NLIS algorithm.
CO2_IASB_NLIS (L2)	9.1	4-6	02.2013 – 12.2021	Mid-tropospheric CO_2 mixing ratios as retrieved from IASI/Metop-B using LMD's NLIS algorithm.

Table 2: Overview CH_4 products. “CRD#” indicates the Climate Data Record (CDR) Number. Level 2 (L2) products contains information for each individual satellite footprint (ground pixel) whereas Level 3 (L3) products are gridded /averaged spatially and temporally.

Product ID (Level)	Version	CDR#	Temporal coverage	Comments
CH4_GOS_OCFP (L2)	7.3	4-6	04.2009 – 12.2021	XCH_4 from GOSAT as retrieved with Univ. Leicester’s OCFP algorithm.
CH4_GOS_OCPR (L2)	9.0	4-6	04.2009 – 12.2021	XCH_4 from GOSAT as retrieved with Univ. Leicester’s OCPR algorithm.
CH4_GO2_SRFP (L2)	2.0.0	6	02.2019 – 12.2021	XCH_4 from GOSAT-2 as retrieved with SRON’s SRFP (RemoTeC) algorithm.
CH4_GO2_SRPR (L2)	2.0.0	6	02.2019 – 12.2021	XCH_4 from GOSAT-2 as retrieved with SRON’s SRPR (RemoTeC) algorithm.
XCH4_EMMA (L2)	4.4	6	01.2003 – 12.2021	Merged L2 XCH_4 product using Univ. Bremen’s EMMA algorithm.
XCH4_OBS4MIPS (L3)	4.4	6	01.2003 – 12.2021	Merged L3 XCH_4 product in OBS4MIPS format.
CH4_IASA_NLIS (L2)	9.1	4-6	07.2007 – 08.2021	Mid-tropospheric CH_4 mixing ratios as retrieved from IASI/Metop-A using LMD’s NLIS algorithm.
CH4_IASB_NLIS (L2)	9.1	4-6	02.2013 – 12.2021	Mid-tropospheric CH_4 mixing ratios as retrieved from IASI/Metop-B using LMD’s NLIS algorithm.

Executive summary

CO_2 and CH_4 are important climate-relevant atmospheric gases, so-called greenhouse gases (GHG). Because of their important role for climate, they are classified as Essential Climate Variables (ECVs). The ECV GHG as formulated by GCOS (Global Climate Observing System) is defined as follows: “Retrievals of greenhouse gases, such as CO_2 and CH_4, of sufficient quality to estimate regional sources and sinks” (GCOS-154). This definition contains already the main application of these atmospheric data products, namely to use them (in combination with appropriate modelling) to obtain (improved) information on their (primarily surface) sources and sinks.

In this document the retrieval algorithms are described, which are used to generate satellite-derived atmospheric carbon dioxide (CO_2) and methane (CH_4) 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/).

These satellite-derived greenhouse gas (GHG) data products are:

- Column-average dry-air mixing ratios (mole fractions) of CO_2 and CH_4, denoted XCO_2 (in parts per million, ppm) and XCH_4 (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO_2 (in ppm) and CH_4 (in ppb).

The C3S GHG data products are generated - or have been generated in the past - from the satellite instruments SCIAMACHY onboard ENVISAT, TANSO-FTS/GOSAT, TANSO-FTS-2/GOSAT-2 (XCO_2 and XCH_4 products) and AIRS and IASI (mid/upper troposphere products). Products from SCIAMACHY and AIRS have been generated in pre-cursor projects and no updates are generated within this project; the corresponding GHG products are available via the Copernicus Climate Data Store (CDS, https://cds.climate.copernicus.eu/). Note however that SCIAMACHY products are used as input for the generation of the four merged products that are produced here: XCO2_EMMA, XCO2_OBS4MIPS, XCH4_EMMA, and XCH4_OBS4MIPS. For the products XCO2_EMMA and XCO2_OBS4MIPS also Level 2 products from NASA’s OCO-2 mission have been used as input products (see also Reuter et al., 2020).

All data products are available in NetCDF format. All products except the two (XCO_2 and XCH_4) Level 3 Obs4MIPs format products are Level 2 products. The XCO_2 and XCH_4 Level 2 products correspond to individual satellite sensors but are also available as merged multi-sensor products (the so-called EMMA products).

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/).

The first GHG data set - Climate Data Record 1 (CDR1) - covered the time period 2003-2016 and had been delivered to ECMWF in 2017. That data set and its documentation has been made available via the C3S CDS in mid 2018. The second data set - Climate Data Record 2 (CDR2) - covered the time period 2003-2017 and has been made available for the C3S CDS in October 2018. This document is an update of document ATBD for the latest CDR data set CDR6 covering the time period 2002-2021.

The algorithms which are used to retrieve XCO_2 and/or XCH_4 from SCIAMACHY/ENVISAT, TANSO-FTS/GOSAT/GOSAT-2 and OCO-2 are based on radiative transfer modelling of the observed radiance spectra. Using Optimal Estimation (OE) or Least-Squares retrieval methods, parameters called state vector elements (or fit parameters) are iteratively adjusted until a good match is obtained between the modelled and the observed radiance spectra. Among these state vector elements are those elements which permit to compute the desired parameters XCO_2 and XCH_4. These state vector elements are parameters describing the CO_2 and CH_4 vertical profile or directly correspond to their vertical column. Other state vector elements consider effects which are also required for accurate modelling of the observed spectra such as parameters related to surface reflection, atmospheric scattering (aerosols, clouds), water vapor and temperature vertical profiles and surface pressure. Output of these algorithms are not only the quantities XCO_2 and XCH_4 but also their uncertainty and their altitude sensitivity (averaging kernels) as well as a quality flag, which indicated if the retrieval is considered reliable or not. The quality flag reflects the quality of the spectral fit but is also determined by a number of other aspects such as the values of certain state vector elements (or combinations of them). These algorithms are typically relatively slow as line absorption as well as multiple scattering needs to be considered for the radiative transfer simulations, which cover a quite large spectral region. In contrast, the algorithm used to retrieve mid/upper tropospheric CO_2 and CH_4 mixing ratios from the IASI instruments on the Metop satellite series is very fast as it is based on the neuronal network method.

This document is structured as follows: In Sect. 1 an overview of the satellites instruments is provided. Sect. 2 addresses input data and auxiliary data as used by the retrieval algorithms. The main section is Sect. 3, where the retrieval algorithms are described. Output data are addressed in Sect. 4. An acknowledgment is given in Sect. 5. Note that this document is the MAIN ATBD document providing only a very short overview about the retrieval algorithms. Details on each algorithm are provided in separate ANNEXes (see Sect. 6):

- **ANNEX A:** ATBD for XCO2 and XCH4 Level 2 products CO2_GOS_OCFP, CH4_GOS_OCFP and CH4_GOS_OCPR retrieved from GOSAT using University of Leicester's "full physics" (FP) and "proxy" (PR) retrieval algorithms
- **ANNEX B**: ATBD for XCO_2 and XCH_4 Level 2 products CO2_GO2_SRFP and CH4_GO2_SRFP retrieved using SRON's FP retrieval algorithm from GOSAT-2
- **ANNEX C**: ATBD for XCH_4 Level 2 product CH4_GO2_SRPR retrieved using SRON's PR retrieval algorithm from GOSAT-2
- **ANNEX D**: ATBD for merged multi-sensor / multi-algorithms Level 2 and Level 3 products XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS and XCH4_OBS4MIPS as generated using University of Bremen's algorithms
- **ANNEX E**: ATBD for IASI CO_2 and CH_4 Level 2 mid/upper troposphere products generated at LMD (includes also information on AIRS CO_2 mid-tropospheric products generated in a previous project)

1. Instruments

1.1 Instruments for XCO_2 and/or XCH_4 retrievals

Satellite radiance observations in the Near Infrared / Short Wave Infrared (NIR/SWIR) spectral region in nadir (downward looking) observation viewing mode are sensitive to atmospheric CO_2 and CH_4 concentration changes with good sensitivity down to the Earth's surface (because solar radiation reflected at the Earth's surface is observed). These measurements permit to obtain "total column information" but do not permit to obtain (detailed) information on the vertical profiles of CO_2 and CH_4. The CO_2 and CH_4 products derived from these satellites are column-averaged dry-air mixing ratios (more precisely: mole fractions) of CO_2 and CH_4 denoted XCO_2 (e.g., in ppm) and XCH_4 (e.g., in ppb).

In the following, several satellite instruments are briefly described which are used / can be used to generate XCO_2 and/or XCH_4 data products.

Currently data from three of these instruments – SCIAMACHY/ENVISAT, TANSO-FTS/GOSAT/GOSAT-2 and OCO-2 - have been used to generate the XCO_2 and XCH_4 data products described in this document. Data products from additional sensors may be added in the future.

1.1.1 SCIAMACHY onboard ENVISAT

SCIAMACHY (SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY) was a spectrometer on ESA's ENVISAT satellite (2002-2012). SCIAMACHY (Burrows et al., 2005; Bovensmann et al., 1999) covers the spectral region from the ultra-violet to the SWIR spectral region (240 nm - 2380 nm) at moderate spectral resolution (0.2 nm - 1.5 nm) and observes the Earth's atmosphere in various viewing geometries (nadir, limb and solar and lunar occultation). For a good general overview on SCIAMACHY see also https://en.wikipedia.org/wiki/SCIAMACHY. SCIAMACHY permits the retrieval of XCO_2 (e.g., Reuter et al., 2011; Schneising et al., 2011) and XCH_4 (e.g., Schneising et al., 2011; Frankenberg et al., 2011) from the appropriate spectral regions in the SWIR (around 1.6 µm) and the NIR (O_2 A-band at 760 nm used to obtain the dry-air column using the know dry-air mixing ratio of atmospheric oxygen). The ground pixel size is typically 30 km along track times 60 km across track and the swath width is about 960 km. There are no across-track gaps between the ground pixels but there are gaps along-track as SCIAMACHY operates only part of the time (approx. 50%) in nadir observation mode.

1.1.2 TANSO-FTS onboard GOSAT and GOSAT-2

TANSO-FTS is a Fourier-Transform-Spectrometer (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_2, CH_4 and O_2 absorption bands in the NIR and SWIR spectral region as needed for accurate XCO_2 and XCH_4 retrieval (in addition GOSAT also covers a large part of the Thermal Infrared (TIR) spectral region). The spectral resolution of TANSO-FTS is much higher compared to SCIAMACHY and the ground pixels are smaller (10 km compared to several 10 km for SCIAMACHY). However, in contrast to SCIAMACHY, 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/.

GOSAT-2 (Suto et al., 2021) was successfully launched on 29 October 2018. GOSAT-2 XCO_2 and XCH_4 retrievals are now also included in the C3S GHG CDR.

Concerning XCO_2 and XCH_4 retrieval from GOSAT and GOSAT-2 see also Noël et al., 2021 and 2022.

1.1.3 OCO-2

NASA's Orbiting Carbon Observatory 2 (OCO-2) mission (Crisp et al., 2004; Boesch et al., 2011) has been successfully launched in July 2014. The OCO-2 Project primary science objective is to collect the first space-based measurements of atmospheric carbon dioxide with the precision, resolution and coverage needed to characterize its sources and sinks and quantify their variability over the seasonal cycle. During its two-year mission, OCO-2 will fly in a sun-synchronous, near-polar orbit with a group of Earth-orbiting satellites with synergistic science objectives whose ascending node crosses the equator near 13:30 hours Mean Local Time (MLT). Near-global coverage of the sunlit portion of Earth is provided in this orbit over a 16-day (233-revolution) repeat cycle. OCO-2's single instrument incorporates three high-resolution grating spectrometers, designed to measure the near-infrared absorption of reflected sunlight by carbon dioxide and molecular oxygen. OCO-2 covers similar spectral bands as SCIAMACHY and GOSAT but OCO-2 has much smaller ground pixels (km scale) but the swath width is much smaller (approx. 10 km) compared to SCIAMACHY. OCO-2 delivers XCO_2 but not XCH_4. Details on OCO-2 are also given on https://oco.jpl.nasa.gov/.

1.2 Instruments for mid-tropospheric mixing ratios of CO_2 and CH_4

Satellite radiance observations in the thermal infrared (TIR) spectral region in nadir (downward looking) observation viewing mode are sensitive to atmospheric CO_2 and CH_4 mixing ratio changes in the mid and upper tropospheric region. They can thus be interpreted in terms of integrated mid-tropospheric columns, with typical sensitivity between 5 and 12 km.

Mid-tropospheric columns of CO_2 can be retrieved from hyperspectral infrared sounders such as AIRS and IASI (Chédin et al., 2003; Crevoisier et al., 2003) using non-linear inference scheme (Crevoisier et al., 2009a). Products can be validated using aircraft measurements, mostly from the Comprehensive Observation Network for TRace gases by AIrLiner (CONTRAIL) program (Machida et al., 2008; Matsueda et al. 2008).

Mid-tropospheric columns of CH_4 can be retrieved from the hyperspectral infrared sounder IASI (Crevoisier et al., 2003, 2013) using non-linear inference scheme (Crevoisier et al., 2009b). Products can be validated using aircraft measurements, from the Comprehensive Observation Network for TRace gases by AIrLiner (CONTRAIL) program (Machida et al., 2008; Matsueda et al. 2008) and the HIAPER Pole-to-Pole Observations (HIPPO) project (Wofsy et al., 2012), as well as from balloon measurements from AirCores (Membrive et al., 2016).

In the following, the 2 hyperspectral infrared sounders AIRS and IASI are briefly described.

1.2.1 AIRS

The Atmospheric Infrared Sounder (AIRS) is a polar orbiting nadir-viewing high-resolution infrared sounder operating in a cross-track-scanning mode. It was launched onboard the EOS Aqua satellite in May 2002, with two operational microwave sounders, AMSU and HSB, and is operational since September 2002. It is a high-spectral resolution, grating multispectral infrared sounder with 2378 channels. Its spectral domain ranges from 650 cm^{-1} to 2665 cm^{-1} (15.4 µm and 3.8 µm), with a spectral resolving power of 1200 (i.e., a spectral resolution ranging from 0.5 cm^{-1} to 2 cm^{-1}). This domain is divided into three spectral bands, from 650 to 1135 cm^{-1}, from 1215 to 1615 cm^{-1} and from 2180 to 2665 cm^{-1}. AIRS cross-track scanning is 1650 km and covers 70% of the earth every day. The instantaneous field of view (IFOV) is sampled by 3×3 circular pixels whose ground resolution is 13 km at nadir. Measurements from the three instruments are analyzed jointly to filter out the effects of clouds from the IR data in order to derive clear-column air-temperature profiles and surface temperatures with high vertical resolution and accuracy (1 K per 1 km layer in the troposphere).

1.2.2 IASI

The Infrared Atmospheric Sounding Interferometer (IASI) is a high resolution Fourier Transform Spectrometer based on a Michelson Interferometer coupled to an integrated imaging system that measures infrared radiation emitted from the Earth. Developed by the Center National d'Etudes

Spatiales (CNES) in collaboration with the European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT), IASI was launched in October 2006 onboard the polar orbiting Meteorological Operational Platform (Metop-A), in September 2012 onboard Metop-B, and in November 2018 onboard Metop-C. IASI provides 8461 spectral samples, ranging from 645 cm^{-1} to 2760 cm^{-1} (15.5 µm and 3.6 µm), with a spectral sampling of 0.25 cm^{-1}, and a spectral resolution of 0.5 cm^{-1} after apodisation, i.e., after application of a method to reduce the spectral resolution (‘Level 1c’ spectra). IASI is an across track scanning system, whose swath width is of 2200 km, allowing global coverage twice a day. The IFOV is sampled by 2×2 circular pixels whose ground resolution is 12 km at nadir. IASI has demonstrated the possibility to retrieve or detect several chemistry and climate variables from hyperspectral infrared observation: for instance, water vapour (H_2O), carbon dioxide (CO_2), carbon monoxide (CO), methane (CH_4), ozone (O_3), sulfur dioxide (SO_2), hydrogen sulfide (H_2S), ammonia (NH_3), nitric acid (HNO_3), volatile organic compounds (VOCs) and aerosols (Hilton et al., 2012; Clarisse et al., 2011) on regional and global scales. IASI enables the monitoring of key gases for climate and atmospheric chemistry in near real time and has also highlighted the benefit of high-performance infrared sounders for numerical weather prevision (NWP) applications.

2. Inputs and auxiliary data

Details on input and auxiliary data are given in specific Annexes (see Sect. 6.).

3. Algorithms

3.1 Algorithms for products CO2_GOS_OCFP, CH4_GOS_OCFP and CH4_GOS_OCPR (ANNEX A)

The products CO2_GOS_OCFP, CH4_GOS_OCFP and CH4_GOS_OCPR are XCO_2 and XCH_4 Level 2 products as retrieved from GOSAT using retrieval algorithms developed at the University of Leicester, UK.

For details see the separate ATBD provided as ANNEX A.

3.2 Algorithms for products CO2_GO2_SRFP and CH4_GO2_SRFP (ANNEX B)

The products CO2_GO2_SRFP and CH4_GO2_SRFP are XCO_2 and XCH_4 Level 2 products as retrieved from GOSAT-2 using "Full Physics" (FP) algorithms developed at SRON, The Netherlands.

For details see the separate ATBD provided as ANNEX B.

3.3 Algorithm for product CH4_GO2_SRPR (ANNEX C)

The product CH4_GO2_SRPR is a XCH_4 Level 2 product as retrieved from GOSAT-2 using a (light path) "Proxy" (PR) algorithm developed at SRON, The Netherlands.

For details see the separate ATBD provided as ANNEX C.

3.4 Algorithms for XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, XCH4_OBS4MIPS (ANNEX D)

The products XCO2_EMMA and XCH4_EMMA are merged multi-sensor XCO_2 and XCH_4 Level 2 products generated using the Ensemble Median Algorithm (EMMA, Reuter et al., 2013) developed at University of Bremen, Germany. The OBS4MIPS product are derived from the EMMA products (via "gridding"). They have a spatial resolution of $5^o x 5^o$ and monthly time resolution.

For details see the separate ATBD provided as ANNEX D.

3.5 Algorithms for CO_2 and CH_4 IASI and AIRS products (ANNEX E)

The IASI products are mid-tropospheric CO_2 and CH_4 mixing ratios and the AIRS product is a mid-tropospheric CO_2 mixing ratio product. These products are retrieved using algorithms developed at LMD/CNRS, France.

For details see the separate ATBD provided as ANNEX E.

4. Output data

The output data products are (see also Buchwitz et al., 2013b, 2017, 2017b):

- Column-average dry-air mixing ratios (mole fractions) of CO_2 and CH_4, denoted XCO_2 (in parts per million, ppm) and XCH_4 (in parts per billion, ppb).
- Mid/upper tropospheric mixing ratios of CO_2 and CH_4.

Carbon dioxide and methane are important atmospheric greenhouse gases (e.g., IPCC 2013) but despite their importance our knowledge on their various and variable natural and anthropogenic sources and sinks has significant gaps (e.g., IPCC 2013; Ciais et al., 2014; 2015; Kirschke et al., 2013; Nisbet et al., 2014, and references given therein). A purpose of the satellite data products described in this document is to contribute to enhancing our knowledge on the CO_2 and CH_4 sources and sinks (via appropriate (inverse) modelling).

Carbon dioxide and methane are so-called Essential Climate Variables (ECVs) and the need to monitor them has been clearly identified including the definition of key requirements (e.g., GCOS-154, GCOS-200). In recent years several satellite-derived ECV data products have been generated in particular in the framework of the Climate Change Initiative (CCI) of ESA (e.g., Hollmann et al., 2013) including CO_2 and CH_4 (e.g., Buchwitz et al., 2013a, 2016, 2017, 2017b).

These satellite-derived CO_2 and CH_4 data products are used for a number of (primarily scientific) applications, e.g.,

- to improve our knowledge on the various natural and anthropogenic (surface) sources and sinks of these important greenhouse gases (GHG) (see, e.g., Alexe et al., 2015; Chevallier et al., 2014, 2016a, 2016b; Cressot et al, 2014; Detmers et al., 2015; Guerlet et al., 2013; Houweling et al., 2015; McNorton et al., 2016; Pandey et al., 2016; Reuter et al., 2014b, 2017; Schneising et al., 2014b; Turner et al., 2015, 2016, and references given therein)
- to monitor the global distribution of CO_2 and CH_4 (e.g., Buchwitz et al., 2007, 2016, 2017b; Schneising et al., 2011; Frankenberg et al., 2011; Massart et al., 2016)
- to improve our knowledge on emission ratios, e.g., for biomass burning (e.g., Ross et al., 2013; Parker et al., 2016)
- for comparisons with (chemistry) climate models (e.g., Shindell et al., 2013; Hayman et al., 2014; Lauer et al., 2017) and other models (e.g., Schneising et al., 2014a; Parker et al., 2016)

The following tables (3-5) provide an overview of the CO_2 and CH_4 data products.

Table 3 - Overview XCO_2 data products.

Product ID	Level	Sensor(s)	(Planned) Availability	Comments
CO2_GOS_OCFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017 Dec. 2019: 2009-2018 Dec. 2020: 2009-2019 Jul. 2021: 2009-mid 2020 Dec. 2022: 2009-2021	Univ. Leicester's "Full Physics" (FP) algorithm
CO2_GO2_SRFP	2	GOSAT-2	Dec. 2022: 2019-2021	SRON's "Full Physics" (FP) algorithm
XCO2_EMMA	2	Merged SCIAMACHY, GOSAT, OCO-2	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017 Dec. 2019: 2003-2018 Dec. 2020: 2003-2019 Jul. 2021: 2003-mid 2020 Dec. 2022: 2003-2021	Univ. Bremen's Level 2 merging algorithm
XCO2_OBS4MIPS	3	Merged SCIAMACHY, GOSAT, OCO-2	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017 Dec. 2019: 2003-2018 Dec. 2020: 2003-2019 Jul. 2021: 2003-mid 2020 Dec. 2022: 2003-2021	Gridded EMMA product in Obs4MIPs format

Table 4 - Overview XCH_4 data products.

Product ID	Level	Sensor(s)	(Planned) Availability	Comments
CH4_GOS_OCPR	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017 Dec. 2019: 2009-2018 Dec. 2020: 2009-2019 Jul. 2021: 2009-mid 2020 Dec. 2022: 2009-2021	Univ. Leicester's "Proxy" (PR) algorithm
CH4_GOS_OCFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017 Dec. 2019: 2009-2018 Dec. 2020: 2009-2019 Jul. 2021: 2009-mid 2020 Dec. 2022: 2009-2021	Univ. Leicester's "Full Physics" (FP) algorithm
CH4_GO2_SRPR	2	GOSAT-2	Dec. 2022: 2019-2021	SRON's "Proxy" (PR) algorithm
CH4_GO2_SRFP	2	GOSAT-2	Dec. 2022: 2019-2021	SRON's "Full Physics" (FP) algorithm
XCH4_EMMA	2	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017 Dec. 2019: 2003-2018 Dec. 2020: 2003-2019 Jul. 2021: 2003-mid 2020 Dec. 2022: 2003-2021	Univ. Bremen's Level 2 merging algorithm
XCH4_OBS4MIPS	3	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017 Dec. 2019: 2003-2018 Dec. 2020: 2003-2019 Jul. 2021: 2003-mid 2020 Dec. 2022: 2003-2021	Gridded EMMA product in Obs4MIPs format

Table 5 - Overview mid/upper troposphere CO_2 and CH_4 data products.

Product ID	Level	Sensor(s)	(Planned) Availability	Comments
CO2_IASA_NLIS	2	IASI / Metop-A	Oct. 2017: 2007-2015 Dec. 2020: 2007-2019 Jul. 2021: 2007 - 11.2020 Dec. 2022: 2007-07.2021	IASI-A: Nominal operation ended July 2021.
CH4_IASA_NLIS	2	IASI / Metop-A	Oct. 2017: 2007-2015 Dec. 2020: 2007-2019 Jul. 2021: 2007 – 11.2020 Dec. 2022: 2007-07.2021	IASI-A: Nominal operation ended July 2021.
CO2_IASB_NLIS	2	IASI / Metop-B	Oct. 2017: 2013-2016 Oct. 2018: 2013-2017 Dec. 2019: 2013-2018 Dec. 2020: 2013-2019 Jul. 2021: 2013 – 11.2020 Dec. 2022: 2013-2021	
CH4_IASB_NLIS	2	IASI / Metop-B	Oct. 2017: 2013-2016 Oct. 2018: 2013-2017 Dec. 2019: 2013-2018 Dec. 2020: 2013-2019 Jul. 2021: 2013 – 11.2020 Dec. 2022: 2013-2021	

The output data consist for each Level 2 product of one daily NetCDF file. These files contain for each single satellite footprint (ground pixel) the main parameter (e.g., XCO_2 or XCH_4 or mid-tropospheric CO_2 or CH_4), its uncertainty, its averaging kernel and its *a priori* profile in addition to other information (most notable geolocation and time information: latitude, longitude, time).

In addition, two Level 3 products are generated: one for XCO_2 and one for XCH4. Each product is stored in a single file covering the entire time series, i.e., there is one file for XCO_2 and one file for XCH_4.

For details on the output format please see the corresponding Product User Guide and Specification (PUGS) document [D5].

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We also acknowledge the availability of OCO-2 Level 1 and Level 2 (XCO_2) data products from NASA, which have been used for the generation on the XCO2_EMMA and XCO2_OBS4MIPS products. These products also include OCO-2 XCO_2 retrieved at Univ. Bremen with the FOCAL algorithm. The FOCAL activities would not have been possible without funding from University of Bremen, from the EU H2020 projects CHE (grant agreement ID: 776186) and VERIFY (Grant agreement ID: 776810), from ESA via project GHG-CCI+ and from EUMETSAT project FOCAL-CO2M.

Finally, yet importantly we acknowledge the availability of TCCON data via the TCCON data archive (https://tccondata.org/).

6. List of ANNEXes

The ANNEXes to this main document are the following ANNEXes A – E:

6.1 ANNEX A: ATBD for products CO2_GOS_OCFP, CH4_GOS_OCFP and CH4_OCPR

Describes algorithms for GOSAT XCO_2 and XCH_4 Level 2 products generated by University of Leicester, UK.

6.2 ANNEX B: ATBD for products CO2_GO2_SRFP and CH4_GO2_SRFP

Describes algorithms for GOSAT-2 XCO_2 and XCH_4 Full Physics (FP) Level 2 products generated by SRON, The Netherlands.

6.3 ANNEX C: ATBD for product CH4_GO2_SRPR

Describes the algorithm for GOSAT-2 XCH_4 Proxy (PR) Level 2 product generated by SRON, The Netherlands.

6.4 ANNEX D: ATBD for XCO2_EMMA, XCH4_EMMA, XCO2_OBS4MIPS, XCH4_OBS4MIPS

Describes algorithms for multi-sensor merged XCO_2 and XCH_4 Level 2 ("EMMA") products and gridded Level 3 ("OBS4MIPS") products (as derived from the EMMA products) generated by University of Bremen, Germany.

6.5 ANNEX E: ATBD for IASI and AIRS CO_2 and CH_4 products

Describes algorithms for mid-tropospheric CO_2 and CH_4 products from the IASI instrument series and from AIRS generated by LMD/CNRS, France.

These ANNEXes and the corresponding data products are / will be available via the Copernicus Climate Data Store (CDS):
[*https://cds.climate.copernicus.eu/#!/home*](https://cds.climate.copernicus.eu/#!/home)

See also Copernicus Climate Change Service (C3S):
[*https://climate.copernicus.eu/*](https://climate.copernicus.eu/)

pdf versions of all documents (including previous versions) are (also) available from
[*https://www.iup.uni-bremen.de/carbon_ghg/cg_data.html#C3S_GHG*](https://www.iup.uni-bremen.de/carbon_ghg/cg_data.html#C3S_GHG)

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