ECMWF COPERNICUS REPORT

Copernicus Climate Change Service

Algorithm Theoretical Basis Document (ATBD) – Main document for data set CDR2 (2003-2017)

C3S_312a_Lot6_IUP-UB – Greenhouse Gases

Issued by: Michael Buchwitz, University of Bremen,

Institute of Environmental Physics (IUP)

Date: 16/10/2018

Ref: C3S_D312a_Lot6.2.1.2-v2_ATBD_MAIN_v2.0

Official reference number service contract: 2016/C3S_312a_Lot6_IUP-UB/SC1

Contributors

INSTITUTE OF ENVIRONMENTAL PHYSICS (IUP), UNIVERSITY OF BREMEN, BREMEN, GERMANY
(IUP)
M. Buchwitz
M. Reuter
O. Schneising-Weigel

SRON NETHERLANDS INSTITUTE FOR SPACE RESEARCH, UTRECHT, THE NETHERLANDS
(SRON)
I. Aben
R. G. Detmers
O. P. Hasekamp

UNIVERSITY OF LEICESTER, LEICESTER, UK
(UoL)
H. Boesch
J. Anand

CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE (CNRS), LABORATOIRE DE METEOROLOGIE DYNAMIQUE (LMD), PALAISEAU, FRANCE
(LMD/CNRS)
C. Crevoisier
R. Armante

Table of Contents

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

Related documents

Reference ID	Document
D1	**GCOS-154:** Global Climate Observing System (GCOS), SYSTEMATIC OBSERVATION REQUIREMENTS FOR SATELLITE-BASED PRODUCTS FOR CLIMATE, 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)", Prepared by World Meteorological Organization (WMO), Intergovernmental Oceanographic Commission, United Nations Environment Programme (UNEP), International Council for Science, Doc.: GCOS 154, link: https://www.wmo.int/pages/prog/gcos/Publications/gcos-154.pdf, 2010.
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, link: http://www.esa-ghg-cci.org/?q=webfm_send/344, 2016.
D4	**TRD GHG, 2017:** Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Target Requirement Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO_2 and CH_4) data products (project C3S_312a_Lot6), Version 1.3, 20-October-2017, pp. 53, 2017.

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
GOME	Global Ozone Monitoring Experiment
GMES	Global Monitoring for Environment and Security
GOSAT	Greenhouse Gases Observing Satellite
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
OCO	Orbiting Carbon Observatory
OE	Optimal Estimation
PBL	Planetary Boundary Layer
ppb	Parts per billion
ppm	Parts per million
PR	(light path) PRoxy retrieval method
PVIR	Product Validation and Intercomparison Report
QA	Quality Assurance
QC	Quality Control
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
SWIR	Short Wava Infra Red
TANSO	Thermal And Near infrared Sensor for carbon Observation
TANSO-FTS	Fourier Transform Spectrometer on GOSAT
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

Table 1 lists some general definitions relevant for this document.

Table 1: General definitions.

Item	Definition
XCO_2	Column-average dry-air mixing ratio (mole fraction) of CO_2
XCH_4	Column-average dry-air mixing ratio (mole fraction) of CH_4
L1	Level 1 satellite data product: geolocated radiance (spectra)
L2	Level 2 satellite-derived data product: Here: CO_2 and CH_4 information for each ground-pixel
L3	Level 3 satellite-derived data product: Here: Gridded CO_2 and CH_4 information, e.g., 5 deg times 5 deg, monthly
L4	Level 4 satellite-derived data product: Here: Surface fluxes (emission and/or uptake) of CO_2 and CH_4

Scope of 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 project C3S_312a_Lot6 led by University of Bremen, Germany.

Within this 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_312a_Lot 6 satellite-derived 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).

An overview about the products is given in Table 2 for the CO_2 products and in Table 3 for the CH_4 products.

Requirements on data quality are formulated in the corresponding Target Requirement Document (TRD) (*TRD GHG, 2017*).

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 only the main ATBD providing an overview about all product and their underlying retrieval algorithms. Details on each algorithm, or group of similar algorithms, are described in a set of ANNEXes to this document.

Table 2: Overview CO_2 products. "CRD#" indicates the Climate Data Record Number. CRD1 has been released in 2017 and CDR2 in 2018. Level 2 (L2) products contains information for each individual satellite footprint (ground pixel) whereas Level 3 (L3) products are gridded /averaged spatially and temporally. If CDR# is 1&2 then this means that the product has not been updated for CDR2, i.e., the product is still the latest version.

Product ID (Level)	**Version**	**CDR#**	**Temporal coverage**	**Comments**
CO2_SCI_BESD (L2)	02.01.02	1&2	01.2003 – 03.2012	XCO_2 from SCIAMACHY as retrieved with Univ. Bremen's BESD algorithm. Brokered from GHG-CCI.
CO2_SCI_WFMD (L2)	4.0	1&2	10.2002 – 04.2012	XCO_2 from SCIAMACHY as retrieved with Univ. Bremen's WFMD algorithm. Brokered from GHG-CCI.
CO2_GOS_OCFP (L2)	7.1 7.2	1 2	04.2009 – 12.2016 04.2009 – 12.2017	XCO_2 from GOSAT as retrieved with Univ. Leicester's OCFP algorithm.
CO2_GOS_SRFP (L2)	2.3.8 2.3.8	1 2	04.2009 – 12.2016 04.2009 – 12.2017	XCO_2 from GOSAT as retrieved with SRON's SRFP (RemoTeC) algorithm. Year 2017 has been added for CDR2.
XCO2_EMMA (L2)	3.0 3.1	1 2	01.2003 – 12.2016 01.2003 – 12.2017	Merged L2 XCO_2 product using Univ. Bremen's EMMA algorithm.
XCO2_OBS4MIPS (L3)	3 3.1	1 2	01.2003 – 12.2016 01.2003 – 12.2017	Merged L3 XCO_2 product in OBS4MIPS format.
CO2_AIRS_NLIS (L2)	3.0	1&2	04.2003 – 07.2007	Mid-tropospheric CO_2 mixing ratios as retrieved from AIRS using LMD's NLIS algorithm. Brokered from GHG-CCI.
CO2_IASA_NLIS (L2)	8.0	1&2	7.2007 – 05.2015	Mid-tropospheric CO_2 mixing ratios as retrieved from IASI/Metop-A using LMD's NLIS algorithm.
CO2_IASB_NLIS (L2)	4.0 4.2	1 2	2.2013 – 12.2016 2.2013 – 12.2017	Mid-tropospheric CO_2 mixing ratios as retrieved from IASI/Metop-B using LMD's NLIS algorithm.

Table 3: Overview CH_4 products. “CRD#” indicates the Climate Data Record Number. CRD1 has been released in 2017 and CDR2 in 2018. Level 2 (L2) products contains information for each individual satellite footprint (ground pixel) whereas Level 3 (L3) products are gridded /averaged spatially and temporally. If CDR# is 1&2 then this means that the product has not been updated for CDR2, i.e., the product is still the latest version.

Product ID (Level)	Version	CDR#	Temporal coverage	Comments
CH4_SCI_WFMD (L2)	4.0	1&2	10.2002 – 12.2011	XCH_4 from SCIAMACHY as retrieved with Univ. Bremen’s WFMD algorithm. Brokered from GHG-CCI.
CH4_SCI_IMAP (L2)	7.2	1&2	01.2003 – 04.2012	XCH_4 from SCIAMACHY as retrieved with SRON/JPL’s IMAP algorithm. Brokered from GHG-CCI.
CH4_GOS_OCPR (L2)	7.0 7.2	1 2	04.2009 – 12.2016 04.2009 – 12.2017	XCH_4 from GOSAT as retrieved with Univ. Leicester’s OCPR algorithm.
CH4_GOS_SRPR (L2)	2.3.8 2.3.9	1 2	04.2009 – 12.2016 04.2009 – 12.2017	XCH_4 from GOSAT as retrieved with SRON’s SRPR (RemoTeC) algorithm.
CH4_GOS_OCFP (L2)	7.1 7.2	1 2	04.2009 – 12.2016 04.2009 – 12.2017	XCH_4 from GOSAT as retrieved with Univ. Leicester’s OCFP algorithm.
CH4_GOS_SRFP (L2)	2.3.8 2.3.8	1 2	04.2009 – 12.2016 04.2009 – 12.2017	XCH_4 from GOSAT as retrieved with SRON’s SRFP (RemoTeC) algorithm. Year 2017 has been added for CDR2.
XCH4_EMMA (L2)	3.0 3.1	1 2	01.2003 – 12.2016 01.2003 – 12.2017	Merged L2 XCH_4 product using Univ. Bremen’s EMMA algorithm.
XCH4_OBS4MIPS (L3)	3 3.1	1 2	01.2003 – 12.2016 01.2003 – 12.2017	Merged L3 XCH_4 product in OBS4MIPS format.
CH4_IASA_NLIS (L2)	8.0	1&2	7.2007 – 05.2015	Mid-tropospheric CH_4 mixing ratios as retrieved from IASI/Metop-A using LMD’s NLIS algorithm.
CH4_IASB_NLIS (L2)	8.1 8.1	1 2	2.2013 – 12.2016 2.2013 – 12.2017	Mid-tropospheric CH_4 mixing ratios as retrieved from IASI/Metop-B using LMD’s NLIS algorithm. Year 2017 has been added for CDR2.

Executive summary

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 C3S_312a_Lot6 project of the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/).

These satellite-derived 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).

These data products are generated from the satellite instruments SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT (XCO_2 and XCH_4 products) and AIRS and IASI (mid/upper tropospheric CO_2 and CH_4 products). All data products are available as Level 2 (individual sounding, i.e., per ground pixels) products in NetCDF format. The XCO_2 and XCH_4 Level 2 products are available for individual sensors but also as merged multi-sensor products. In addition, also merged Level 3 (i.e., gridded) products in Obs4MIPs format are available for the XCO_2 and XCH_4 products.

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.

Both gases, CO_2 and CH_4, have a long lifetime in the atmosphere. As a consequence of this fact and related human emissions the atmospheric concentrations of these gases are relatively high (currently about 400 ppm for CO_2 and 1.8 ppm for CH_4) compared to other atmospheric trace gases. As a result of this even a moderate to strong (surface) source or sink typically only results in a relatively small local or regional change (enhancement or depletion relative to the surrounding region) in their vertical columns or their mid/upper tropospheric concentration. The observational requirements are therefore very demanding in particular with respect to random and systematic errors and stability (*GCOS-154; GCOS-200; TRD GHG, 2017*).

Because of their long lifetime and atmospheric transport, elevated (or depleted) atmospheric CO_2 and CH_4 concentrations can be higher (or lower) relative to the background far away from the surface source (or sink), which has emitted (or taken up) these atmospheric gases. In order to obtain source/sink information from the atmospheric observations it is therefore required to take atmospheric transport (and esp. for methane also atmospheric chemistry) into account and to consider the exact time and location of the atmospheric observations. As a consequence, the most relevant data products are the Level 2 (L2) products, which contain detailed information on time and location (and other information such as averaging kernels) for each individual satellite ground pixel. The requirements as formulated in the Target Requirement Document (*TRD GHG, 2017*) are, therefore, mostly L2 requirements.

The C3S_312a_Lot6 project is essentially the (pre-)operational continuation of the research and development (R&D) pre-cursor project GHG-CCI (http://www.esa-ghg-cci.org/) of ESA's Climate Change Initiative (CCI). The main goal of the C3S_312a_Lot6 project is to extend (in time) the data base of GHG-CCI pre-cursor data products.

The first C3S_312a_Lot6 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) - coveres the time period 2003-2017 and has be made available for the C3S CDS in October 2018. This document is an update of the ATBD for data set CDR2.

The algorithms which are used to retrieve XCO_2 and XCH_4 from SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT are based on radiative transfer modelling of the observed radiance spectra. Using Optimal Estimation (OE) or Least-Squares 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 the MAIN ATBD document. It only provides a very short overview about the data products and their underlying retrieval algorithms. Details on each algorithm are provided in separate ANNEXes (except for the OBS4MIPS products; the algorithms to generate these products are described in this document):

- **ANNEX A**: ATBD for XCO_2 and XCH_4 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_GOS_SRFP and CH4_GOS_SRFP retrieved using SRON's FP retrieval algorithm
- **ANNEX C**: ATBD for XCH_4 Level 2 product CH4_GOS_SRPR retrieved using SRON's PR retrieval algorithm
- **ANNEX D**: ATBD for Level 2 merged multi-sensor products XCO2_EMMA and XCH4_EMMA generated using University of Bremen's EMMA algorithm
- **ANNEX E**: ATBD for IASI CO_2 and CH_4 Level 2 mid/upper troposphere products generated at LMD

1. Overview data products and instruments

In this section an overview of the data products - specified in terms of variable, its property, processing level(s) and instrument(s) - is given.

The data products are (see also *Buchwitz et al., 2013b, 2016, 2017*):

- 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*).

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; Bergamaschi 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, 2016b; 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*)

In the following sub-sections an overview about the satellite-derived CO_2 and CH_4 data products is given.

1.1 Column-average mixing ratios of CO_2 and CH_4 (XCO_2 and XCH_4)

1.1.1 Overview

Satellite radiance observations in the Near Infrared / Short Wave Infrared (NIR/SWIR) spectral region in nadir (downlooking) 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 shortly described which are used / can be used to generate XCO_2 and/or XCH_4 data products.

1.1.2 Instruments

In this section a short overview about relevant satellite instruments is given.

Currently data from two of these instruments – SCIAMACHY and TANSO-FTS - have been used to generate the Level 2 XCO_2 and XCH_4 data products described and assessed in this document. Data products from additional sensors may be added in the future.

1.1.2.1 SCIAMACHY/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.

1.1.2.2 TANSO-FTS/GOSAT

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 also 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/.

1.1.2.3 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/.

1.1.2.4 TanSat

The Chinese TanSat satellite (https://en.wikipedia.org/wiki/TanSat) has been successfully launched in December 2016. The TanSat satellite and instrument is very similar as OCO-2. As OCO-2, TanSat delivers XCO_2 but not XCH_4. At the time of writing only few details on the achieved in-orbit XCO_2 performance of TanSat are available.

1.1.2.5 Sentinel-5-Precursor (S5P)

ESA's Sentinel-5-Precursor (S5P) mission (*Veefkind et al, 2012*) has been launched in 2017. S5P permits XCH_4 retrievals (*Butz et al., 2012, Hu et al., 2018*) at about 7 km and using a wide swath of about 2600 km. Details on S5P can also be found on https://earth.esa.int/web/guest/missions/esa-future-missions/sentinel-5P.

1.1.2.6 Other instruments

Several other satellites are expected to be launched in the future, e.g., the GOSAT follow-on GOSAT-2 for XCO_2 and XCH_4, the active laser-based mission MERLIN (Methane Remote Sensing Lidar Mission, see https://de.wikipedia.org/wiki/Merlin_(Satellit)) for XCH_4 and NASA's recently approved geostationary GeoCARB mission. It can also be expected that in the future other satellites will be launched which permit also to obtain detailed global information on anthropogenic CO_2 emissions (e.g., *Ciais et al., 2015*), for example a satellite like CarbonSat (*Bovenmann et al., 2010; Buchwitz et al., 2013b; Pillai et al., 2016*) or even a CarbonSat-like constellation (*Velazco et al., 2011*).

1.1.3 XCO_2

As explained, XCO_2 is the column-averaged dry-air mixing ratio (mole fraction) of atmospheric CO_2. A XCO_2 value of, for example, 400 ppm at a given location means that about 400 CO_2 molecules are present in the atmosphere above that location per one million air molecules excluding water molecules.

XCO_2 can be retrieved from instruments such as SCIAMACHY and TANSO-FTS/GOSAT using Optimal Estimation (*Rodgers, 2000*) or DOAS (*Buchwitz et al., 2000*) retrieval algorithms as shown in various publications (e.g., *Buchwitz et al., 2005; Butz et al., 2011; Cogan et al., 2011; Reuter et al., 2011; 2013; Schneising et al., 2011; Yoshida et al., 2013*).

These products are validated using Total Carbon Column Observing Network (TCCON) (*Wunch et al., 2010, 2011, 2015*) XCO_2 ground based observations (e.g., *Dils et al., 2014*).

1.1.4 XCH_4

As explained, XCH_4 is the column-averaged dry-air mixing ratio (mole fraction) of atmospheric CH_4. A XCH_4 value of, for example, 1800 ppb at a given location means that about 1800 CH_4 molecules are present in the atmosphere above that location per one billion air molecules excluding water molecules.

XCH_4 can be retrieved from instruments such as SCIAMACHY and TANSO-FTS/GOSAT using Optimal Estimation (*Rodgers, 2000*) or DOAS (*Buchwitz et al., 2000*) retrieval algorithms as shown in various publications (e.g., *Buchwitz et al., 2005; Butz et al., 2011; Frankenberg et al., 2011; Schneising et al., 2011; Parker et al., 2011; Scheper et al., 2012; Yoshida et al., 201*3).

These products are validated using Total Carbon Column Observing Network (TCCON) (*Wunch et al., 2010, 2011, 2015*) XCH_4 ground based observations (e.g., *Dils et al., 2014*).

1.1.5 List of XCO_2 and XCH_4 data products

Table 4 and Table 5 list the XCO_2 and XCH_4 data products, respectively.

As can be seen from Table 4, for each individual sensor Level 2 XCO_2 product two products are generated using two different retrieval algorithms (OCFP is University of Leicester's Full Physics (FP) algorithm and SRFP is SRON's FP retrieval algorithm, also known as RemoTeC).

The availability of more than one product ("mini ensemble") permits to give more confidence in terms of robustness of results, e.g., with respect to findings related to the sources and sinks of CO_2 (e.g., *Reuter et al., 2014b, 2017*).

Products with comment « Existing GHG-CCI product » are the latest versions of Level 2 products, which have been generated in the framework of the GHG-CCI project (http://www.esa-ghg-cci.org/). They existed already prior to C3S and are available from the GHG-CCI website (http://www.esa-ghg-cci.org/ -> CRDP (Data)) including documentation (in particular Product User Guide (PUG, one document per product / product family), Algorithm Theoretical Basis Document (ATBD, one document per product / product family), Product Validation and Intercomparison Report (PVIR, single document covering all products)). They have been used within project C3S_312a_Lot6 to generate the merged Level 2 and Level 3 EMMA and OBS4MIPS products but the individual sensor L2 products have not been regenerated. They have been provided for C3S « as is » and are available via the C3S CDS.

As can be seen from Table 5, for each individual sensor Level 2 XCH_4 product four products will be generated from GOSAT using four different retrieval algorithms using two « Full Physics » (FP) and two « Proxy » (PR) algorithms. For a discussion of FP versus PR algorithms see, for example, *Schepers et al., 2012*. Each type of algorithm has different advantages and disadvantages. Typically, the PR products contain much more data as quality filtering can be less strict but the PR algorithms use a CO_2 model to correct for XCO_2 variations. FP products contain less data points but the advantage of this product is that it is independent of a CO_2 model.

Table 4 - 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	
CO2_GOS_SRFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017	
CO2_SCI_BESD	2	SCIAMACHY	Oct. 2017: 2003-2012	Existing GHG-CCI product
CO2_SCI_WFMD	2	SCIAMACHY	Oct. 2017: 2002-2012	Existing GHG-CCI product
XCO2_EMMA	2	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017	
XCO2_OBS4MIPS	3	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017	

Table 5 - 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	
CH4_GOS_SRPR	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017	
CH4_GOS_OCFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017	
CH4_GOS_SRFP	2	GOSAT	Oct. 2017: 2009-2016 Oct. 2018: 2009-2017	
CH4_SCI_WFMD	2	SCIAMACHY	Oct. 2017: 2002-2011	Existing GHG-CCI product
CH4_SCI_IMAP	2	SCIAMACHY	Oct. 2017: 2003-2012	Existing GHG-CCI product
XCH4_EMMA	2	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 201 : 2003-2017	
XCH4_OBS4MIPS	3	Merged SCIAMACHY & GOSAT	Oct. 2017: 2003-2016 Oct. 2018: 2003-2017	

1.2 Mid-tropospheric mixing ratios of CO_2 and CH_4

1.2.1 Overview

Satellite radiance observations in the thermal infrared (TIR) spectral region in nadir (downlooking) 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.

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

1.2.2 Instruments

1.2.2.1 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).

1.2.2.2 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), and in September 2012 onboard Metop-B. A third IASI will be launched 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 ('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 vapor (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.

1.2.3 CO_2

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*).

1.2.4 CH_4

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*).

1.2.5 List of mid-tropospheric CO_2 and CH_4 data products

Table 6 lists the CO_2 and CH_4 mid/upper troposphere data products.

The product with comment « Existing GHG-CCI product » is the latest versions of AIRS CO_2 Level 2 products, which has been generated in the framework of the GHG-CCI project (http://www.esa-ghg-cci.org/). This product exists and is available from the GHG-CCI website (http://www.esa-ghg-cci.org/ -> CRDP (Data)). It has been provided for C3S essentially « as is » but converted (from ASCII) to NetCDF format (all products listed in Table 6 are available in NetCDF format).

Table 6 - 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	
CH4_IASA_NLIS	2	IASI / Metop-A	Oct. 2017: 2007-2015	
CO2_IASB_NLIS	2	IASI / Metop-B	Oct. 2017: 2013-2016 Oct. 2018: 2013-2017	
CH4_IASB_NLIS	2	IASI / Metop-B	Oct. 2017: 2013-2016 Oct. 2018: 2013-2017	
CO2_AIR_NLIS	2	AIRS	Oct. 2017: 2003-2007	Existing GHG-CCI product

2. 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 (see Sect. 10).

3. Algorithms for products CO2_GOS_SRFP and CH4_GOS_SRFP (ANNEX B)

The products CO2_GOS_SRFP and CH4_GOS_SRFP are XCO_2 and XCH_4 Level 2 products as retrieved from GOSAT using "Full Physics" (FP) algorithms developed at SRON, The Netherlands.

For details see the separate ATBD provided as ANNEX B (see Sect. 10).

4. Algorithm for product CH4_GOS_SRPR (ANNEX C)

The product CH4_GOS_SRPR is a XCH_4 Level 2 product as retrieved from GOSAT using a (light path) "Proxy" (PR) algorithm developed at SRON, The Netherlands.

For details see the separate ATBD provided as ANNEX C (see Sect. 10).

5. Algorithms for products XCO2_EMMA and XCH4_EMMA (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.

For details see the separate ATBD provided as ANNEX D (see Sect. 10).

6. Algorithms for CO_2 and CH_4 IASI products (ANNEX E)

The IASI products are mid-tropospheric CO_2 and CH_4 mixing ratios retrieved using algorithms developed at LMD/CNRS, France.

For details see the separate ATBD provided as ANNEX E (see Sect. 10).

7. Algorithms for OBS4MIPS XCO_2 and XCH_4 products

The Obs4MIPs XCO_2 and XCH_4 products are multi-sensor merged L3 (Level 3) products generated using algorithms developed at the University of Bremen, Germany.

The data basis for the Obs4MIPs products are the EMMA Level 2 XCO_2 and XCH_4 data products described in ANNEX D and correspond to arithmetic 5°x5° monthly averages. In order to keep the contribution of instrumental noise small in the L3 products, only grid boxes with standard errors of the mean being smaller than 1.6 ppm (XCO_2) and 12 ppb (XCH_4) are considered.

In addition to the average XCO_2 and XCH_4 values, also the number of L2 values, the standard deviation of L2 values, and the overall uncertainty σ are computed per L3 grid box. In this context, the overall uncertainty is computed by

$$\sigma = \sqrt{\sigma_m + \sigma_i}$$

whereas σ_m represents the standard error of the mean computed from the individual stochastic sounding uncertainties and σ_i the inter-algorithm spread computed by EMMA (see ANNEX D).

8. Algorithms for existing GHG-CCI products

In this section a short overview about those algorithm is given which have been used (in the past) to generate products which are not regenerated within C3S but made available for C3S and whose products are used as input for the merged Level 2 (EMMA) and Level 3 (OBS4MIPS) products.

8.1 Algorithm for CO2_SCI_BESD product

Product: XCO_2
Level: 2
Sensor: SCIAMACHY/ENVISAT
Algorithm type: Optimal Estimation
Reference:

- Reuter, M., H. Bovensmann, M. Buchwitz, J. P. Burrows, B. J. Connor, N. M. Deutscher, D. W. T. Griffith, J. Heymann, G. Keppel-Aleks, J. Messerschmidt, J. Notholt, C. Petri, J. Robinson, O. Schneising, V. Sherlock, V. Velazco, T. Warneke, P. O. Wennberg, and D. Wunch: "Retrieval of atmospheric CO2 with enhanced accuracy and precision from SCIAMACHY: Validation with FTS measurements and comparison with model results" J. Geophys. Res., doi: 10.1029/2010JD015047, 2011.

Details: CO2_SCI_BESD ATBD:

- Reuter, M, et al., Algorithm Theoretical Basis Document Version 5 (ATBDv5) - The Bremen Optimal Estimation DOAS (BESD) algorithm for the retrieval of XCO2; ESA Climate Change Initiative (CCI) for the Essential Climate Variable (ECV) Greenhouse Gases (GHG), pp. 83, 2017. Link: http://www.esa-ghg-cci.org/webfm_send/338

8.2 Algorithm for CO2_SCI_WFMD and CH4_SCI_WFMD products

Product: XCO_2 and XCH_4
Level: 2
Sensor: SCIAMACHY/ENVISAT
Algorithm type: Least-squares DOAS
Reference:

- Schneising, O., Buchwitz, M., Reuter, M., Heymann, J., Bovensmann, H., and Burrows, J. P.: Long-term analysis of carbon dioxide and methane column-averaged mole fractions retrieved from SCIAMACHY, Atmos. Chem. Phys., 11, 2863-2880, doi:10.5194/acp-11-2863-2011, 2011.

Details: CO2_SCI_WFMD & CH4_SCI_WFMD ATBD:

- Schneising, O., et al., Algorithm Theoretical Basis Document (ATBD) - SCIAMACHY WFM-DOAS (WFMD) XCO_2 and XCH_4 for the Essential Climate Variable (ECV) Greenhouse Gases (GHG), 15.May 2016, pp. 37, 2016. Link: http://www.esa-ghg-cci.org/index.php?q=webfm_send/334

8.3 Algorithm for CH4_SCI_IMAP product

Product: XCH_4
Level: 2
Sensor: SCIAMACHY/ENVISAT
Algorithm type: Optimal Estimation DOAS
Reference:

- Frankenberg, C., Aben, I., Bergamaschi, P., et al., Global column-averaged methane mixing ratios from 2003 to 2009 as derived from SCIAMACHY: Trends and variability, J. Geophys. Res., doi:10.1029/2010JD014849, 2011.

Details: CH4_SCI_IMAP ATBD:

- Frankenberg, C., et al., Algorithm Theoretical Basis Document Version 5 (ATBDv5) – The SRON IMAP-DOAS retrieval of XCH4, v7.2 for the Essential Climate Variable (ECV) Greenhouse Gases (GHG), 28. August 2016, pp. 115, 2016. Link: http://www.esa-ghg-cci.org/?q=webfm_send/377

8.4 Algorithm for CO2_AIR_NLIS product

Product: Mid tropospheric CO_2 mixing ratio
Level: 2
Sensor: AIRS
Algorithm type: Neuronal Network
Reference:

- Crevoisier, C., S. Heilliette, A. Chédin, S. Serrar, R. Armante, and N. A. Scott, Midtropospheric CO2 concentration retrieval from AIRS observations in the tropics, Geophys. Res. Lett., 31, L17106, doi:10.1029/2004GL020141, 2004.

Note that a dedicated ATBD does not exist for this brokered product. This product is generated with the NLIS algorithm. The NLIS algorithm as applied to IASI is described in ANNEX E, see Sect. 10.5.

References

Alexe et al., 2015: Alexe, M., P. Bergamaschi, A. Segers, R. Detmers, A. Butz, O. Hasekamp, S. Guerlet, R. Parker, H. Boesch, C. Frankenberg, R. A. Scheepmaker, E. Dlugokencky, C. Sweeney, S. C. Wofsy, and E. A. Kort, Inverse modeling of CH4 emissions for 2010–2011 using different satellite retrieval products from GOSAT and SCIAMACHY, Atmos. Chem. Phys., 15, 113–133, doi:10.5194/acp-15-113-2015, 2015.

Bergamaschi et al., 2009: Bergamaschi, P., Frankenberg, C., Meirink, J. F., Krol, M., Villani, M. G., Houweling, S., Dentener, F., Dlugokencky, E. J., Miller, J. B., Gatti, L. V., Engel, A., and Levin, I.: Inverse modeling of global and regional CH_4 emissions using SCIAMACHY satellite retrievals, J. Geophys. Res., 114, D22301, doi:10.1029/2009JD012287, 2009.

Bergamaschi et al., 2013: Bergamaschi, P., Houweling, H., Segers, A., et al., Atmospheric CH4 in the first decade of the 21st century: Inverse modeling analysis using SCIAMACHY satellite retrievals and NOAA surface measurements, J. Geophys. Res., 118, 7350-7369, doi:10.1002/jrgd.50480, 2013.

Boesch et al., 2011: Boesch, H., D. Baker, B. Connor, D. Crisp, and C. Miller, Global characterization of CO_2 column retrievals from shortwave-infrared satellite observations of the Orbiting Carbon Observatory-2 mission, Remote Sensing, 3 (2), 270-304, 2011.

Bovensmann et al., 1999: Bovensmann, H., Burrows, J. P., Buchwitz, M., Frerick, J., Noël, S., Rozanov, V. V., Chance, K. V., Goede, A. H. P. (1999), SCIAMACHY - Mission objectives and measurement modes, J. Atmos. Sci., 56 (2), 127-150, 1999.

Bovensmann et al., 2010: Bovensmann, H., Buchwitz, M., Burrows, J. P., Reuter, M., Krings, T., Gerilowski, K., Schneising, O., Heymann, J., Tretner, A., and Erzinger, J.: A remote sensing technique for global monitoring of power plant CO_2 emissions from space and related applications, Atmos. Meas. Tech., 3, 781-811, 2010.

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

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

Buchwitz et al., 2007: Buchwitz, M., O. Schneising, J. P. Burrows, H. Bovensmann, M. Reuter, J. Notholt, First direct observation of the atmospheric CO_2 year-to-year increase from space, Atmos. Chem. Phys., 7, 4249-4256, 2007.

Buchwitz et al., 2013a: Buchwitz, M., M. Reuter, O. Schneising, H. Boesch, S. Guerlet, B. Dils, I. Aben, R. Armante, P. Bergamaschi, T. Blumenstock, H. Bovensmann, D. Brunner, B. Buchmann, J. P. Burrows, A. Butz, A. Chédin, F. Chevallier, C. D. Crevoisier, N. M. Deutscher, C. Frankenberg, F. Hase, O. P. Hasekamp, J. Heymann, T. Kaminski, A. Laeng, G. Lichtenberg, M. De Mazière, S. Noël, J. Notholt, J. Orphal, C. Popp, R. Parker, M. Scholze, R. Sussmann, G. P. Stiller, T. Warneke, C. Zehner, A. Bril, D. Crisp, D. W. T. Griffith, A. Kuze, C. O'Dell, S. Oshchepkov, V. Sherlock, H. Suto, P. Wennberg, D. Wunch, T. Yokota, Y. Yoshida, The Greenhouse Gas Climate Change Initiative (GHG-

CCI): comparison and quality assessment of near-surface-sensitive satellite-derived CO_2 and CH_4 global data sets, *Remote Sensing of Environment*, doi:10.1016/j.rse.2013.04.024, http://authors.elsevier.com/sd/article/S0034425713003520, 2013.

Buchwitz et al., 2013b: Buchwitz, M., Reuter, M., Bovensmann, H., Pillai, D., Heymann, J., Schneising, O., Rozanov, V., Krings, T., Burrows, J. P., Boesch, H., Gerbig, C., Meijer, Y., and Loescher, A.: Carbon Monitoring Satellite (CarbonSat): assessment of atmospheric CO_2 and CH_4 retrieval errors by error parameterization, Atmos. Meas. Tech., 6, 3477-3500, 2013.

Buchwitz et al., 2015: Buchwitz, M., Reuter, M., Schneising, O., Boesch, H., Guerlet, S., Dils, B., Aben, I., Armante, R., Bergamaschi, P., Blumenstock, T., Bovensmann, H., Brunner, D., Buchmann, B., Burrows, J.P., Butz, A., Chédin, A., Chevallier, F., Crevoisier, C.D., Deutscher, N.M., Frankenberg, C., Hase, F., Hasekamp, O.P., Heymann, J., Kaminski, T., Laeng, A., Lichtenberg, G., De Mazière, M., Noël, S., Notholt, J., Orphal, J., Popp, C., Parker, R., Scholze, M., Sussmann, R., Stiller, G.P., Warneke, T., Zehner, C., Bril, A., Crisp, D., Griffith, D.W.T., Kuze, A., O'Dell, C., Oshchepkov, S., Sherlock, V., Suto, H., Wennberg, P., Wunch, D., Yokota, T., Yoshida, Y., The Greenhouse Gas Climate Change Initiative (GHG-CCI): comparison and quality assessment of near-surface-sensitive satellite-derived CO2 and CH4 global data sets. Remote Sens. Environ. 162:344–362, http://dx.doi.org/10.1016/j.rse.2013.04.024, 2015.

Buchwitz et al., 2016: Buchwitz, M., Reuter, M., Schneising, O., Hewson, W., Detmers, R. G., Boesch, H., Hasekamp, O. P., Aben, I., Bovensmann, H., Burrows, J. P., Butz, A., Chevallier, F., Dils, B., Frankenberg, C., Heymann, J., Lichtenberg, G., De Mazière, M., Notholt, J., Parker, R., Warneke, T., Zehner, C., Griffith, D. W. T., Deutscher, N. M., Kuze, A., Suto, H., and Wunch, D.:, Global satellite observations of column-averaged carbon dioxide and methane: The GHG-CCI XCO_2 and XCH_4 CRDP3 data, Remote Sensing of Environment (in press), Special Issue on Essential Climate Variables, DOI: 10.1016/j.rse.2016.12.027, (link: http://dx.doi.org/10.1016/j.rse.2016.12.027), 2016.

Buchwitz et al., 2016a: Buchwitz, M.; Reuter, M.; Aben, I.; Boesch, H.; Butz, A.; Detmers, R.G.; Frankenberg, C.; Hasekamp, O.P.; Parker, R.; Schneising, O.; Somkuti, P., ESA Greenhouse Gases Climate Change Initiative (GHG-CCI): Merged SCIAMACHY and GOSAT Level 3 gridded atmospheric column-average methane (XCH_4) product in Obs4MIPs format, Centre for Environmental Data Analysis, 10 October 2016, doi:10.5285/C965E4AC-D2AF-4BAA-9E99-A234E9BA0193, link: http://www.esa-ghg-cci.org/?q=webfm_send/331, pp. 11, 2016.

Buchwitz et al., 2017: ESA Climate Change Initiative (CCI) Product Validation and Intercomparison Report (PVIR) for the Essential Climate Variable (ECV) Greenhouse Gases (GHG) for data set Climate Research Data Package No. 4 (CRDP#4), Version 5.0, 9. Feb. 2017, link: http://www.esa-ghg-cci.org/?q=webfm_send/352, 2017.

Buchwitz et al., 2017a: Buchwitz, M.; Reuter, M.; Aben, I.; Boesch, H.; Butz, A.; Detmers, R.G.; Frankenberg, C.; Hasekamp, O.P.; Parker, R.; Schneising, O.; Somkuti, P., ESA Greenhouse Gases Climate Change Initiative (GHG-CCI): Merged SCIAMACHY and GOSAT Level 3 gridded atmospheric column-average methane (XCH_4) product in Obs4MIPs format version 2 (CRDP#4), Technical Note, link: http://www.esa-ghg-cci.org/?q=webfm_send/349, pp. 11, 1 February 2017, 2017.

Burrows et al., 1995: Burrows, J. P., Hölzle, E., Goede, A. P. H., Visser, H., and Fricke, W., SCIAMACHY—Scanning Imaging Absorption Spectrometer for Atmospheric Chartography, Acta Astronaut., 35(7), 445–451, doi:10.1016/0094-5765(94)00278-t, 1995.

Butz et al., 2011: Butz, A., Guerlet, S., Hasekamp, O., et al., Toward accurate CO_2 and CH_4 observations from GOSAT, *Geophys. Res. Lett.*, doi:10.1029/2011GL047888, 2011.

Butz et al., 2012: Butz, A., Galli, A., Hasekamp, O., Landgraf, J., Tol, P., and Aben, I.: Remote Sensing of Environment, TROPOMI aboard Sentinel-5 Precursor : Prospective performance of CH_4 retrievals for aerosol and cirrus loaded atmospheres, 120, 267-276, doi:10.1016/j.rse.2011.05.030, 2012.

Chédin et al. 2003: Chédin, A., Saunders, R., Hollingsworth, A., Scott, N. A., Matricardi, M., Etcheto, J., Clerbaux, C., Armante, R. and Crevoisier, C.: The feasibility of monitoring CO_2 from high resolution infrared sounders. J. Geophys. Res., 108, ACH 6-1–6-19, doi: 10.1029/2001JD001443, 2003.

Chevallier et al., 2005: Chevallier, F., R. J. Engelen, and P. Peylin, The contribution of AIRS data to the estimation of CO_2 sources and sinks. Geophys. Res. Lett., 32, L23801, doi:10.1029/ 2005GL024229, 2005.

Chevallier et al., 2007: Chevallier, F., F.-M. Bréon, and P. J. Rayner, Contribution of the Orbiting Carbon Observatory to the estimation of CO_2 sources and sinks: Theoretical study in a variational data assimilation framework. J. Geophys. Res., 112, D09307, doi:10.1029/2006JD007375, 2007.

Chevallier et al., 2009a: Chevallier, F., R. J. Engelen, C. Carouge, T. J. Conway, P. Peylin, C. Pickett-Heaps, M. Ramonet, P. J. Rayner and I. Xueref-Remy, AIRS-based vs. surface-based estimation of carbon surface fluxes. J. Geophys. Res., 114, D20303, doi:10.1029/2009JD012311, 2009.

Chevallier et al., 2009b: Chevallier, F., S. Maksyutov, P. Bousquet, F.-M. Bréon, R. Saito, Y. Yoshida, and T. Yokota, On the accuracy of the CO_2 surface fluxes to be estimated from the GOSAT observations. Geophys. Res. Lett., 36, L19807, doi:10.1029/2009GL040108, 2009.

Chevallier et al., 2010: Chevallier, F., Feng, L., Boesch, H. Palmer, P., and Rayner, P., On the impact of transport model errors for the estimation of CO_2 surface fluxes from GOSAT observations, Geophys. Res. Let., 37, L21803, 2010.

Chevallier et al., 2014: Chevallier, F., Palmer, P.I., Feng, L., Boesch, H., O'Dell, C.W., Bousquet, P., Towards robust and consistent regional CO_2 flux estimates from in situ and space-borne measurements of atmospheric CO_2, Geophys. Res. Lett., 41, 1065-1070, DOI: 10.1002/2013GL058772, 2014.

Chevallier et al., 2016b: Chevallier, F., et al., Climate Assessment Report (CAR), ESA Climate Change Initiative (CCI) GHG-CCI project, Version 3, 3 May 2016, link: http://www.esa-ghg-cci.org/?q=webfm_send/318, 2016.

Ciais et al., 2014: Ciais, P., Dolman, A. J., Bombelli, A., et al.: Current systematic carbon cycle observations and needs for implementing a policy-relevant carbon observing system, Biogeosciences, 11, 3547-3602, www.biogeosciences.net/11/3547/2014/, doi:10.5194/bg-11-3547-2014, 2014.

Ciais et al., 2015: Ciais, P., et al.: Towards a European Operational Observing System to Monitor Fossil CO_2 emissions - Final Report from the expert group, http://www.copernicus.eu/main/towards-european-operational-observing-system-monitor-fossil-co2-emissions, pp. 68, October 2015, 2015.

CMUG-RBD, 2010: Climate Modelling User Group Requirements Baseline Document, Deliverable 1.2, Number D1.2, Version 1.3, 2 Nov 2010.

Cogan et al., 2011: Cogan, A. J., Boesch, H., Parker, R. J., et al., Atmospheric carbon dioxide retrieved from the Greenhouse gases Observing SATellite (GOSAT): Comparison with ground-based TCCON observations and GEOS-Chem model calculations, *J. Geophys. Res.*, 117, D21301, doi:10.1029/2012JD018087, 2012.

Corbin et al., 2008: Corbin, K. D., A. S. Denning, L. Lu, J.-W. Wang, and I. T. Baker, Possible representation errors in inversions of satellite CO_2 retrievals, J. Geophys. Res., 113, D02301, doi:10.1029/2007JD008716, 2008.

Cressot et al., 2014: Cressot, C., F. Chevallier, P. Bousquet, et al., On the consistency between global and regional methane emissions inferred from SCIAMACHY, TANSO-FTS, IASI and surface measurements, Atmos. Chem. Phys., 14, 577-592, 2014.

Crevoisier et al., 2004: Crevoisier, C., S. Heilliette, A. Chédin, S. Serrar, R. Armante, and N. A. Scott, Midtropospheric CO_2 concentration retrieval from AIRS observations in the tropics, Geophys. Res. Lett., 31, L17106, doi:10.1029/2004GL020141, 2004.

Crevoisier et al., 2009: Crevoisier, C., Chédin, A., Matsueda, H., et al., First year of upper tropospheric integrated content of CO_2 from IASI hyperspectral infrared observations, *Atmos. Chem. Phys.*, 9, 4797-4810, 2009.

Crevoisier et al. 2009b: Crevoisier, C., Nobileau, D., Fiore, A., Armante, R., Chédin, A., and Scott, N. A.: Tropospheric methane in the tropics – first year from IASI hyperspectral infrared observations, Atmos. Chem. Phys., 9, 6337–6350, doi:10.5194/acp-9-6337-2009, 2009b.

Crevoisier et al., 2013: Crevoisier, C., Nobileau, D., Armante, R., et al., The 2007–2011 evolution of tropical methane in the mid-troposphere as seen from space by MetOp-A/IASI, *Atmos. Chem. Phys.*, 13, 4279-4289, 2013.

Crisp et al., 2004: Crisp, D., Atlas, R. M., Breon, F.-M., Brown, L. R., Burrows, J. P., Ciais, P., Connor, B. J., Doney, S. C., Fung, I. Y., Jacob, D. J., Miller, C. E., O'Brien, D., Pawson, S., Randerson, J. T., Rayner, P., Salawitch, R. S., Sander, S. P., Sen, B., Stephens, G. L., Tans, P. P., Toon, G. C., Wennberg, P. O., Wofsy, S. C., Yung, Y. L., Kuang, Z., Chudasama, B., Sprague, G., Weiss, P., Pollock, R., Kenyon, D., and Schroll, S.: The Orbiting Carbon Observatory (OCO) mission, Adv. Space Res., 34, 700-709, 2004.

Detmers et al., 2015: Detmers, R. G., O. Hasekamp, I. Aben, S. Houweling, T. T. van Leeuwen, A. Butz, J. Landgraf, P. Koehler, L. Guanter, and B. Poulter, Anomalous carbon uptake in Australia as seen by GOSAT, Geophys. Res. Lett., 42, doi:10.1002/2015GL065161, 2015.

Dils et al., 2014: B. Dils, M. Buchwitz, M. Reuter, O. Schneising, H. Boesch, R. Parker, S. Guerlet, I. Aben, T. Blumenstock, J. P. Burrows, A. Butz, N. M. Deutscher, C. Frankenberg, F. Hase, O. P. Hasekamp, J. Heymann, M. De Mazière, J. Notholt, R. Sussmann, T. Warneke, D. Griffith, V. Sherlock, D. Wunch :The Greenhouse Gas Climate Change Initiative (GHG-CCI): Comparative validation of GHG-CCI SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT CO_2 and CH_4 retrieval algorithm products with measurements from the TCCON network, Atmos. Meas. Tech., 7, 1723-1744, 2014.

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, link: http://www.esa-ghg-cci.org/?q=webfm_send/344, 2016.

Frankenberg et al., 2011: Frankenberg, C., Aben, I., Bergamaschi, P., et al., Global column-averaged methane mixing ratios from 2003 to 2009 as derived from SCIAMACHY: Trends and variability, *J. Geophys. Res*., doi:10.1029/2010JD014849, 2011.

GCOS-154: Global Climate Observing System (GCOS), SYSTEMATIC OBSERVATION REQUIREMENTS FOR SATELLITE-BASED PRODUCTS FOR CLIMATE, 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)", Prepared by World Meteorological Organization (WMO), Intergovernmental Oceanographic Commission, United Nations Environment Programme (UNEP), International Council for Science, Doc.: GCOS 154, ink: https://www.wmo.int/pages/prog/gcos/Publications/gcos-154.pdf, 2010.

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.

Guerlet et al., 2013: Guerlet, S., S. Basu, A. Butz, M. Krol, P. Hahne, S. Houweling, O. P. Hasekamp and I. Aben, Reduced carbon uptake during the 2010 Northern Hemisphere summer from GOSAT, Geophys. Res. Lett., doi: 10.1002/grl.50402, 2013.

Hayman et al., 2014: Hayman, G. D., O'Connor, F. M., Dalvi, M., Clark, D. B., Gedney, N., Huntingford, C., Prigent, C., Buchwitz, M., Schneising, O., Burrows, J. P., Wilson, C., Richards, N., Chipperfield, M., Comparison of the HadGEM2 climate-chemistry model against in-situ and SCIAMACHY atmospheric methane data, Atmos. Chem. Phys., 14, 13257-13280, doi:10.5194/acp-14-13257-2014, 2014.

Hollmann et al., 2013: Hollmann, C.J. Merchant, R. Saunders, C. Downy, M. Buchwitz, A. Cazenave, E. Chuvieco, P. Defourny, G. de Leeuw, R. Forsberg, T. Holzer-Popp, F. Paul, S. Sandven, S. Sathyendranath, M. van Roozendael, W. Wagner, The ESA Climate Change Initiative: satellite data records for essential climate variables, Bulletin of the American Meteorological Society (BAMS), 0.1175/BAMS-D-11-00254.1, pp. 12, 2013.

Houweling et al., 2004: Houweling, S., Breon, F.-M., Aben, I., Rödenbeck, C., Gloor, M., Heimann, M. and Ciais, P.: Inverse modeling of CO_2 sources and sinks using satellite data: A synthetic inter-comparison of measurement techniques and their performance as a function of space and time, Atmos. Chem. Phys., 4, 523-538, 2004.

Houweling et al., 2005: Houweling, S., Hartmann, W., Aben, I., Schrijver, H., Skidmore, J., Roelofs, G.-J., and Breon, F.-M.: Evidence of systematic errors in SCIAMACHY-observed CO_2 due to aerosols, Atmos. Chem. Phys., 5, 3003–3013, 2005.

Houweling et al., 2015: Houweling, S., D. Baker, S. Basu, H. Boesch, A. Butz, F. Chevallier, F. Deng, E. J. Dlugokencky, L. Feng, A. Ganshin, O. Hasekamp, D. Jones, S. Maksyutov, J. Marshall, T. Oda, C.W. O'Dell1, S. Oshchepkov, P. I. Palmer, P. Peylin, Z. Poussi, F. Reum, H. Takagi, Y. Yoshida, and R. Zhuravlev, An intercomparison of inverse models for estimating sources and sinks of CO_2 using GOSAT measurements, J. Geophys. Res. Atmos., 120, 5253–5266, doi:10.1002/2014JD022962, 2015.

Hu et al., 2018: Hu, H., J. Landgraf, R. Detmers, T. Borsdorff, J. Aan de Brugh, I. Aben, A. Butz, O. Hasekamp, Toward Global Mapping of Methane With TROPOMI: First Results and Intersatellite Comparison to GOSAT, Geophys. Res. Lett, Vol. 45, Issue 8, 3682-3689, https://doi.org/10.1002/2018GL077259, 2018.

Hungershoefer et al., 2010: Hungershoefer, K., Breon, F.-M., Peylin, P., Chevallier, F., Rayner, P., Klonecki, A., Houweling, S., and Marshall, J., Evaluation of various observing systems for the global monitoring of CO_2 surface fluxes, Atmos. Chem. Phys., 10, 10503-10520, 2010.

IPCC, 2013: Climate Change 2013: The Physical Science Basis, Working Group I Contribution to the Fifth Assessment Report of the Intergovernmental Report on Climate Change, http://www.ipcc.ch/report/ar5/wg1/, 2013.

JCGM, 2008: JCGM/WG 1, Working Group 1 of the Joint Committee for Guides in Metrology, Evalutation of measurement data – Guide to the expression of uncertainty in measurement, http://www.bipm.org/utils/common/documents/jcgm/JCGM_100_2008_E.pdf, 2008.

Kirschke et al., 2013: Kirschke, S., Bousquet, P., Ciais, P., et al.: Three decades of global methane sources and sinks, Nat. Geosci., 6, 813–823, doi:10.1038/ngeo1955, 2013.

Kuze et al., 2009: Kuze, A., Suto, H., Nakajima, M., and Hamazaki, T. (2009), Thermal and near infrared sensor for carbon observation Fourier-transform spectrometer on the Greenhouse Gases Observing Satellite for greenhouse gases monitoring, Appl. Opt., 48, 6716–6733, 2009.

Kuze et al., 2014: Kuze, A., Taylor, T., Kataoka, F., Bruegge, C., Crisp, D., Harada, M., Helmlinger, M., Inoue, M., Kawakami, S., Kikuchi, N., Mitomi, Y., Murooka, J., Naitoh, M., O'Brien, D., O'Dell, C., Ohyama, H., Pollock, H., Schwandner, F., Shiomi, K., Suto, H., Takeda, T., Tanaka, T., Urabe, T., Yokota, T., and Yoshida, Y. (2014), Long-term vicarious calibration of GOSAT short-wave sensors: techniques for error reduction and new estimates of radiometric degradation factors, IEEE T. Geosci. Remote, 52, 3991–4004, doi:10.1109/TGRS.2013.2278696, 2014.

Kuze et al., 2016: Kuze, A., Suto, H., Shiomi, K., Kawakami, S., Tanaka, M., Ueda, Y., Deguchi, A., Yoshida, J., Yamamoto, Y., Kataoka, F., Taylor, T. E., and Buijs, H. L.: Update on GOSAT TANSO-FTS performance, operations, and data products after more than 6 years in space, Atmos. Meas. Tech., 9, 2445-2461, doi:10.5194/amt-9-2445-2016, 2016.

Lauer et al., 2017: Lauer, A., V. Eyring, M. Righi, M. Buchwitz, P. Defourny, M. Evaldsson, P. Friedlingstein, R. de Jeu, G. de Leeuw, A. Loew, C. J. Merchant, B. Müller, T. Popp, M. Reuter, S. Sandven, D. Senftleben, M. Stengel, M. Van Roozendael, S. Wenzel, U, Willén, Benchmarking CMIP5 models with a subset of ESA CCI Phase 2 data using the ESMValTool, Remote Sensing of Environment, DOI: 10.1016/j.rse.2016.12.027, in press, pp. 31, 2017.

Machida et al. 2008: Machida, T., Matsueda, H., Sawa, Y., Nakagawa, Y., Hirotani, K., Kondo, N., Goto, K., Nakazawa, T., Ishikawa, K., and Ogawa, T.: Worldwide measurements of atmospheric CO_2 and other trace gas species using commercial airlines, J. Atmos. Ocean. Tech., 25(10), 1744–1754, doi:10.1175/2008JTECHA1082.1, 2008.

Massart et al., 2016: Massart, S., A. Agustí-Panareda, J. Heymann, M. Buchwitz, F. Chevallier, M. Reuter, M. Hilker, J. P. Burrows, N. M. Deutscher, D. G. Feist, F. Hase, R. Sussmann, F. Desmet, M. K. Dubey, D. W. T. Griffith, R. Kivi, C. Petri, M. Schneider, V. A. Velazco, Ability of the 4-D-Var analysis of the GOSAT BESD XCO_2 retrievals to characterize atmospheric CO_2 at large and synoptic scales, Atmos. Chem. Phys., 16, 1653-1671, doi:10.5194/acp-16-1653-2016, 2016.

Matsueda et al. 2008: Matsueda, H., Machida, T., Sawa, Y., Nakagawa, Y., Hirotani, K., Ikeda, H., Kondo, N., and Goto, K.: Evaluation of atmospheric CO_2 measurements from new flask air sampling of JAL airliner observation, Pap. Meteorol. Geophys., 59, 1–17, 2008.

McNorton et al., 2016: McNorton, J., E. Gloor, C. Wilson, G. D. Hayman, N. Gedney, E. Comyn-Platt, T. Marthews, R. J. Parker, H. Boesch, and M. P. Chipperfield, Role of regional wetland emissions in atmospheric methane variability, Geophys. Res. Lett., 43, doi:10.1002/2016GL070649, 2016.

Meirink et al., 2006: Meirink, J.-F., Eskes, H. J., and Goede, A. P. H., Sensitivity analysis of methane emissions derived from SCIAMACHY observations through inverse modelling, Atmos. Chem. Phys., 6, 1275-1292, 2006.

Membrive et al. 2016: Membrive, O., Crevoisier, C., Sweeney, C., Danis, F., Hertzog, A., Engel, A., Bönisch, H., and Picon, L.: AirCore-HR: A high resolution column sampling to enhance the vertical description of CH_4 and CO_2, Atmos. Meas. Tech. Discuss., doi:10.5194/amt-2016-236, 2016.

Miller et al., 2007: Miller, C. E., Crisp, D., DeCola, P. L., et al.: Precision requirements for space-based XCO2 data, J. Geophys. Res., 112, D10314, doi:10.1029/2006JD007659, 2007.

Nisbet et al., 2014: Nisbet, E., Dlugokencky, E., and Bousquet, P.: Methane on the rise – again, Science, 343, 493–495, doi:10.1126/science.1247828, 2014.

Pandey et al., 2016: Pandey, S., S. Houweling, M. Krol, I. Aben, F. Chevallier, E. J. Dlugokencky, L. V. Gatti, E. Gloor, J. B. Miller, R. Detmers, T. Machida, T. Roeckmann, Inverse modeling of GOSAT-retrieved ratios of total column CH_4 and CO_2 for 2009 and 2010, Atmos. Chem. Phys., 16, 5043–5062, doi:10.5194/acp-16-5043-2016, 2016.

Parker et al., 2011: Parker, R., Boesch, H., Cogan, A., et al., Methane Observations from the Greenhouse gases Observing SATellite: Comparison to ground-based TCCON data and Model Calculations, *Geophys. Res. Lett*., doi:10.1029/2011GL047871, 2011.

Parker et al., 2016: Parker, R. J., H. Boesch, M. J. Wooster, D. P. Moore, A. J. Webb, D. Gaveau, and D. Murdiyarso, Atmospheric CH4 and CO2 enhancements and biomass burning emission ratios derived from satellite observations of the 2015 Indonesian fire plumes, Atmos. Chem. Phys., Atmos. Chem. Phys., 16, 10111-10131, doi:10.5194/acp-16-10111-2016, 2016.

Pillai et al., 2016: Pillai, D., Buchwitz, M., Gerbig, C., Koch, T., Reuter, M., Bovensmann, H., Marshall, J., and Burrows, J. P.: Tracking city CO_2 emissions from space using a high resolution inverse modeling approach: A case study for Berlin, Germany, Atmos. Chem. Phys., 16, 9591-9610, doi:10.5194/acp-16-9591-2016, 2016.

Rayner and O'Brien, 2001: Rayner, P. J., and O'Brien, D.M.: The utility of remotely sensed CO_2 concentration data in surface inversions, Geophys. Res. Lett., 28, 175-178, 2001.

Reuter et al. 2011: Reuter, M., Bovensmann, H., Buchwitz, M., Burrows, J. P., Connor, B. J., Deutscher, N. M., Griffith, D.W. T., Heymann, J., Keppel-Aleks, G., Messerschmidt, J., and et al.: Retrieval of atmospheric CO_2 with enhanced accuracy and precision from SCIAMACHY: Validation with FTS measurements and comparison with model results., Journal of Geophysical Research, 116, doi:10.1029/2010JD015047, URL http://dx.doi.org/10.1029/2010JD015047, 2011.

Reuter et al., 2013: Reuter, M. H. Bösch, H. Bovensmann, A. Bril, M. Buchwitz, A. Butz, J. P. Burrows, C. W. O'Dell, S. Guerlet, O. Hasekamp, J. Heymann, N. Kikuchi, S. Oshchepkov, R. Parker, S. Pfeifer, O. Schneising, T. Yokota, and Y. Yoshida, A joint effort to deliver satellite retrieved atmospheric CO_2 concentrations for surface flux inversions: The ensemble median algorithm EMMA, Atmos. Chem. Phys., 13, 1771-1780, 2013.

Reuter et al., 2014a: Reuter, M., M. Buchwitz, A. Hilboll, A. Richter, O. Schneising, M. Hilker, J. Heymann, H. Bovensmann and J. P. Burrows, Decreasing emissions of NOx relative to CO_2 in East Asia inferred from satellite observations, Nature Geoscience, 28 Sept. 2014, doi:10.1038/ngeo2257, pp.4, 2014.

Reuter et al., 2014b: Reuter, M., M. Buchwitz, M. Hilker, J. Heymann, O. Schneising, D. Pillai, H. Bovensmann, J. P. Burrows, H. Bösch, R. Parker, A. Butz, O. Hasekamp, C. W. O'Dell, Y. Yoshida, C. Gerbig, T. Nehrkorn, N. M. Deutscher, T. Warneke, J. Notholt, F. Hase, R. Kivi, R. Sussmann, T. Machida, H. Matsueda, and Y. Sawa, Satellite-inferred European carbon sink larger than expected, Atmos. Chem. Phys., 14, 13739-13753, doi:10.5194/acp-14-13739-2014, 2014.

Reuter et al., 2016: Reuter, M.; Buchwitz, M.; Aben, I.; Boesch, H.; Butz, A.; Detmers, R.G.; Hasekamp, O.P.; Heymann, J.; Parker, R.; Schneising, O.; Somkuti, P., ESA Greenhouse Gases Climate Change Initiative (GHG_cci): Merged SCIAMACHY and GOSAT Level 3 gridded atmospheric column-average carbon dioxide (XCO_2) product in Obs4MIPs format. Centre for Environmental Data Analysis, 10 October 2016, doi:10.5285/3FAE8371-0CBB-4B21-9EA6-7A1FC293C4A2, link: http://www.esa-ghg-cci.org/?q=webfm_send/330, pp. 11, 2016.

Reuter et al., 2017: Reuter, M., M. Buchwitz, M. Hilker, J. Heymann, H. Bovensmann, J. Burrows, S. Houweling, Y. Liu, R. Nassar, F. Chevallier, P. Ciais, J. Marshall, and M. Reichstein, 2016: How much CO_2 is taken up by the European terrestrial biosphere ?, Bull. Amer. Meteor. Soc. (BAMS), doi:10.1175/BAMS-D-15-00310.1, in press, 2017.

Reuter et al., 2017a: Reuter, M.; Buchwitz, M.; Aben, I.; Boesch, H.; Butz, A.; Detmers, R.G.; Hasekamp, O.P.; Heymann, J.; Parker, R.; Schneising, O.; Somkuti, P., ESA Greenhouse Gases Climate Change Initiative (GHG-CCI): Merged SCIAMACHY and GOSAT Level 3 gridded atmospheric column-average carbon dioxide (XCO_2) product in Obs4MIPs format version 2 (CRDP#4), Technical Note, link: http://www.esa-ghg-cci.org/?q=webfm_send/348 , pp. 11, 1 February 2017, 2017.

Rodgers, 2000: Rodgers C. D.: Inverse Methods for Atmospheric Sounding: Theory and Practice, World Scientific Publishing, 2000.

Ross et al., 2013: Ross, A. N., Wooster, M. J., Boesch, H., Parker, R., First satellite measurements of carbon dioxide and methane emission ratios in wildfire plumes, Geophys. Res. Lett., 40, 1-5, doi:10.1002/grl.50733, 2013.

Schaefer et al., 2016: Schaefer, H., Mikaloff Fletcher, S. E., Veidt, C., Lassey, K. R., Brailsford, G. W., Bromley, T. M., Dlugokencky, E. J., Michel, S. E., Miller, J. B., Levin, I., Lowe, D. C., Martin, R. J., Vaughn, B. H., and White, J. W. C.: A 21st-century shift from fossil-fuel to biogenic methane emissions indicated by $^{13}CH_4$, Science, Vol. 352, Issue 6281, pp. 80-84, doi 10.1126/science.aad2705, 2016.

Shindell et al., 2013: Shindell, D. T., Pechony, O., Voulgarakis, A., et al. (2013), Interactive ozone and methane chemistry in GISS-E2 historical and future climate simulations, Atmos. Chem. Phys., 13, 2653–2689, doi:10.5194/acp-13-2653-2013, 2013.

Schepers et al., 2012: Schepers, D., Guerlet, S., Butz, A., Landgraf, J., Frankenberg, C., Hasekamp, O., Blavier, J.-F., Deutscher, N. M., Griffith, D. W. T., Hase, F., Kyro, E., Morino, I., Sherlock, V., Sussmann, R., Aben, I. (2012), Methane retrievals from Greenhouse Gases Observing Satellite (GOSAT) shortwave infrared measurements: Performance comparison of proxy and physics retrieval algorithms, J. Geophys. Res., 117, D10307, doi:10.1029/2012JD017549, 2012.

Schneising et al., 2011: Schneising, O., Buchwitz, M., Reuter, M., et al., Long-term analysis of carbon dioxide and methane column-averaged mole fractions retrieved from SCIAMACHY, *Atmos. Chem. Phys*., 11, 2881-2892, 2011.

Schneising et al., 2014a: Schneising, O., Reuter, M., Buchwitz, M., Heymann, J., Bovensmann, H., and Burrows, J. P., Terrestrial carbon sink observed from space: variation of growth rates and seasonal cycle amplitudes in response to interannual surface temperature variability, Atmos. Chem. Phys., 14, 133-141, 2014.

Schneising et al., 2014b: Schneising, O., Burrows, J. P., Dickerson, R. R., Buchwitz, M., Reuter, M., Bovensmann, H., Remote sensing of fugitive methane emissions from oil and gas production in North American tight geologic formations, Earth's Future, 2, DOI: 10.1002/2014EF000265, pp. 11, 2014.

TRD GHG, 2017: Buchwitz, M., Aben, I., Anand, J., Armante, R., Boesch, H., Crevoisier, C., Detmers, R. G., Hasekamp, O. P., Reuter, M., Schneising-Weigel, O., Target Requirement Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO_2 and CH_4) data products (project C3S_312a_Lot6), Version 1.3, 20-October-2017, pp. 53, 2017.

Turner et al., 2015: Turner, A. J., D. J. Jacob, K. J. Wecht, J. D. Maasakkers, S. C. Biraud, H. Boesch, K. W. Bowman, N. M. Deutscher, M. K. Dubey, D. W. T. Griffith, F. Hase, A. Kuze, J. Notholt, H. Ohyama, R. Parker, V. H. Payne, R. Sussmann, V. A. Velazco, T. Warneke, P. O. Wennberg, and D. Wunch, Estimating global and North American methane emissions with high spatial resolution using GOSAT satellite data, Atmos. Chem. Phys., 15, 7049-7069, doi:10.5194/acp-15-7049-2015, 2015.

Turner et al., 2016: Turner, A. J., D. J. Jacob, J. Benmergui, S. C. Wofsy, J. D. Maasakkers, A. Butz, O. Hasekamp, and S. C. Biraud, A large increase in U.S. methane emissions over the past decade inferred from satellite data and surface observations, Geophys. Res. Lett., 43, 2218–2224, doi:10.1002/2016GL067987, 2016.

Veefkind et al. 2012: Veefkind, J. P., Aben, I., McMullan, K., Förster, H., De Vries, J., Otter, G., Claas, J., Eskes, H. J., De Haan, J. F., Kleipool, Q., Van Weele, M., Hasekamp, O., Hoogeveen, R., Landgraf, J., Snel, R., Tol, P.,Ingmann, P., Voors, R., Kruizinga, B., Vink, R., Visser, H., and Levelt, P. F.: TROPOMI on the ESA Sentinel-5 Precursor: A GMES mission for global observations of the atmospheric composition for climate, air quality and ozone layer applications. Rem. Sens. Environment, 120:70–83, 2012.

Velazco et al. 2011: Velazco, V. A., Buchwitz, M., Bovensmann, H., Reuter, M., Schneising, O., Heymann, J., Krings, T., Gerilowski, K., and Burrows, J. P.: Towards space based verification of CO2 emissions from strong localized sources: fossil fuel power plant emissions as seen by a CarbonSat constellation, Atmos. Meas. Tech., 4, 2809-2822, 2011.

Wofsy et al. 2012: Wofsy, S. C., Daube, B. C., Jimenez, R., et al.: HIPPO Merged 10-second Meteorology, Atmospheric Chemistry, Aerosol Data (R 20121129), Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, http://dx.doi.org/, 10.3334/CDIAC/hippo 010 (Release 29 November 2012), 2012.

Wunch et al. 2010: Wunch, D., Toon, G. C., Wennberg, P. O., Wofsy, S. C., Stephens, B. B., Fischer, M. L., Uchino, O., Abshire, J. B., Bernath, P., Biraud, S. C., Blavier, J.-F. L., Boone, C., Bowman, K. P., Browell, E. V., Campos, T., Connor, B. J., Daube, B. C., Deutscher, N. M., Diao, M., Elkins, J. W., Gerbig, C., Gottlieb, E., Griffith, D. W. T., Hurst, D. F., Jiménez, R., Keppel-Aleks, G., Kort, E. A., Macatangay, R., Machida, T., Matsueda, H., Moore, F., Morino, I., Park, S., Robinson, J., Roehl, C. M., Sawa, Y., Sherlock, V., Sweeney, C., Tanaka, T., and Zondlo, M. A.: Calibration of the Total Carbon Column Observing Network using aircraft profile data, Atmospheric Measurement Techniques, 3, 1351–1362, doi:10.5194/amt-3-1351-2010, URL http://www.atmos-meas-tech.net/3/1351/2010/, 2010.

Wunch et al. 2011: Wunch, D., Toon, G. C., Blavier, J.-F. L., Washenfelder, R. A., Notholt, J., Connor, B. J., Griffith, D. W. T., Sherlock, V., and Wennberg, P. O.: The Total Carbon Column Observing Network (TCCON), Philosophical Transactions of the Royal Society of London, Series A: Mathematical, Physical and Engineering Sciences, 369, 2087–2112, doi:10.1098/rsta.2010.0240, 2011.

Wunch et al. 2015: Wunch, D., Toon, G.C., Sherlock, V., Deutscher, N.M., Liu, X., Feist, D.G., Wennberg, P.O., The Total Carbon Column Observing Network's GGG2014 Data Version. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA (available at: doi:10.14291/tccon.ggg2014.documentation.R0/1221662), 2015.

Yoshida et al. 2013: Yoshida, Y., Kikuchi, N., Morino, I., Uchino, O., Oshchepkov, S., Bril, A., Saeki, T., Schutgens, N., Toon, G. C., Wunch, D., Roehl, C. M., Wennberg, P. O., Griffith, D. W. T, Deutscher, N. M., Warneke, T., Notholt, J., Robinson, J., Sherlock, V., Connor, B., Rettinger, M., Sussmann, R., Ahonen, P., Heikkinen, P., Kyrö, E., Mendonca, J., Strong, K., Hase, F., Dohe, S., and Yokota, T.: Improvement of the retrieval algorithm for GOSAT SWIR XCO_2 and XCH_4 and their validation using TCCON data, Atmos. Meas. Tech., 6, 1533–1547, doi:10.5194/amt-6-1533-2013, 2013.

9. Acknowledgement

We acknowledge previous funding by the European Space Agency (ESA) via Climate Change Initiative (CCI) project GHG-CCI. This funding significantly enhanced the quality of the retrieval algorithms and related documentation. This resulted in more mature data products as needed for an operational project such as the Copernicus Climate Change Service (C3S). We also acknowledge the availability of GOSAT data products via the ESA GOSAT Third Party Mission (TPM) archive.

We are also very grateful to the GOSAT team in Japan comprising the Japan Aerospace Exploration Agency (JAXA), the National Institute for Environmental Studies (NIES), and the Ministry of the Environment (MOE) for providing access to the GOSAT Level 1 and Level 2 data products via the GOSAT Data Archive Service (GDAS) hosted by NIES.

10. List of ANNEXes

The ANNEXes to this main document are the following ANNEXes A – E valid for data set CDR 2 (2003-2017):

10.1 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.

10.2 ANNEX B: ATBD for products CO2_GOS_SRFP and CH4_GOS_SRFP

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

10.3 ANNEX C: ATBD for product CH4_GOS_SRPR

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

10.4 ANNEX D: ATBD for products XCO2_EMMA and XCH4_EMMA

Describes algorithms for multi-sensor merged XCO_2 and XCH_4 Level 2 products generated by University of Bremen, Germany.

10.5 ANNEX E: ATBD for IASI CO_2 and CH_4 products

Describes algorithms for mid-tropospheric CO2 and CH4 products from the IASI instrument series generated by LMD/CNRS, France.

These ANNEXes and the corresponding data products are available via the Copernicus Climate Data Store (CDS):

https://cds.climate.copernicus.eu/#!/home

See also Copernicus Climate Change Service (C3S):

https://climate.copernicus.eu/

Copernicus Climate Change Service

ECMWF - Shinfield Park, Reading RG2 9AX, UK

Contact: info@copernicus-climate.eu