



# Algorithm Theoretical Basis Document (ATBD) – Main document

## C3S\_312a\_Lot6\_IUP-UB – Greenhouse Gases

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## Table of Contents

<b>History of modifications</b>	<b>6</b>
<b>Related documents</b>	<b>7</b>
<b>Acronyms</b>	<b>8</b>
<b>General definitions</b>	<b>11</b>
<b>Scope of document</b>	<b>12</b>
<b>Executive summary</b>	<b>13</b>
<b>1. Overview data products and instruments</b>	<b>15</b>
<b>1.1 Column-average mixing ratios of CO<sub>2</sub> and CH<sub>4</sub> (XCO<sub>2</sub> and XCH<sub>4</sub>)</b>	<b>16</b>
1.1.1 Overview	16
1.1.2 Instruments	16
1.1.3 XCO <sub>2</sub>	18
1.1.4 XCH <sub>4</sub>	18
1.1.5 List of XCO <sub>2</sub> and XCH <sub>4</sub> data products	19
<b>1.2 Mid-tropospheric mixing ratios of CO<sub>2</sub> and CH<sub>4</sub></b>	<b>21</b>
1.2.1 Overview	21
1.2.2 Instruments	21
1.2.3 CO <sub>2</sub>	22
1.2.4 CH <sub>4</sub>	22
1.2.5 List of mid-tropospheric CO <sub>2</sub> and CH <sub>4</sub> data products	23
<b>2. Algorithms for products CO<sub>2</sub>_GOS_OCFP, CH<sub>4</sub>_GOS_OCFP and CH<sub>4</sub>_GOS_OCPR (ANNEX A)</b>	<b>24</b>
<b>3. Algorithms for products CO<sub>2</sub>_GOS_SRFP and CH<sub>4</sub>_GOS_SRFP (ANNEX B)</b>	<b>24</b>
<b>4. Algorithm for product CH<sub>4</sub>_GOS_SRPR (ANNEX C)</b>	<b>24</b>
<b>5. Algorithms for products XCO<sub>2</sub>_EMMA and XCH<sub>4</sub>_EMMA (ANNEX D)</b>	<b>24</b>
<b>6. Algorithms for CO<sub>2</sub> and CH<sub>4</sub> IASI products (ANNEX E)</b>	<b>25</b>
<b>7. Algorithms for OBS4MIPS XCO<sub>2</sub> and XCH<sub>4</sub> products</b>	<b>26</b>
<b>8. Algorithms for existing GHG-CCI products</b>	<b>27</b>
<b>8.1 Algorithm for CO<sub>2</sub>_SCI_BESD product</b>	<b>27</b>
<b>8.2 Algorithm for CO<sub>2</sub>_SCI_WFMD and CH<sub>4</sub>_SCI_WFMD products</b>	<b>27</b>



<b>8.3 Algorithm for CH<sub>4</sub>_SCI_IMAP product</b>	<b>28</b>
<b>8.4 Algorithm for CO<sub>2</sub>_AIR_NLIS product</b>	<b>28</b>
<b>References</b>	<b>29</b>
<b>9. Acknowledgement</b>	<b>39</b>
<b>10. List of ANNEXes</b>	<b>40</b>
<b>10.1 ANNEX A: ATBD for products CO<sub>2</sub>_GOS_OCFP, CH<sub>4</sub>_GOS_OCFP and CH<sub>4</sub>_OCPR</b>	<b>40</b>
<b>10.2 ANNEX B: ATBD for products CO<sub>2</sub>_GOS_SRF and CH<sub>4</sub>_GOS_SRF</b>	<b>40</b>
<b>10.3 ANNEX C: ATBD for product CH<sub>4</sub>_GOS_SRPR</b>	<b>40</b>
<b>10.4 ANNEX D: ATBD for products XCO<sub>2</sub>_EMMA and XCH<sub>4</sub>_EMMA</b>	<b>40</b>
<b>10.5 ANNEX E: ATBD for IASI CO<sub>2</sub> and CH<sub>4</sub> products</b>	<b>40</b>



## History of modifications

Version	Date	Description of modification	Chapters / Sections
1.0	18-September-2017	New document	All
1.0b	4-October-2017	Information on ATBD for product CH4_SCI_WFMD added to Sect. 8.2 Information on ATBD for product CO2_AIR_NLIS added to Sect. 8.4	Sects. 8.2 and 8.4
1.1	20-October-2017	Link to Copernicus website added TRD reference updated	Sect. 10 Page 7



## Related documents

Reference ID	Document
D1	<b>GCOS-154:</b> 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: <a href="https://www.wmo.int/pages/prog/gcos/Publications/gcos-154.pdf">https://www.wmo.int/pages/prog/gcos/Publications/gcos-154.pdf</a> , 2010.
D2	<b>GCOS-200:</b> The Global Observing System for Climate: Implementation Needs, World Meteorological Organization (WMO), GCOS-200 (GOOS-214), pp. 325, link: <a href="http://unfccc.int/files/science/workstreams/systematic_observation/application/pdf/gcos_ip_10oct2016.pdf">http://unfccc.int/files/science/workstreams/systematic_observation/application/pdf/gcos_ip_10oct2016.pdf</a> , 2016.
D3	<b>ESA-CCI-GHG-URDv2.1:</b> Chevallier, F., et al., User Requirements Document (URD), ESA Climate Change Initiative (CCI) GHG-CCI project, Version 2.1, 19 Oct 2016, link: <a href="http://www.esa-ghg-cci.org/?q=webfm_send/344">http://www.esa-ghg-cci.org/?q=webfm_send/344</a> , 2016.
D4	<b>TRD GHG, 2017:</b> 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 <sub>2</sub> and CH <sub>4</sub> ) 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 <i>neuronal</i> network mid/upper tropospheric CO <sub>2</sub> and CH <sub>4</sub> retrieval algorithm
NOAA	National Oceanic and Atmospheric Administration
Obs4MIPs	Observations for Climate Model Intercomparisons
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 <sub>2</sub>	Column-average dry-air mixing ratio (mole fraction) of CO <sub>2</sub>
XCH <sub>4</sub>	Column-average dry-air mixing ratio (mole fraction) of CH <sub>4</sub>
L1	Level 1 satellite data product: geolocated radiance (spectra)
L2	Level 2 satellite-derived data product: Here: CO <sub>2</sub> and CH <sub>4</sub> information for each ground-pixel
L3	Level 3 satellite-derived data product: Here: Gridded CO <sub>2</sub> and CH <sub>4</sub> 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 <sub>2</sub> and CH <sub>4</sub>



## 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<sub>2</sub>) and methane (CH<sub>4</sub>) 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<sub>2</sub> and CH<sub>4</sub>, denoted XCO<sub>2</sub> (in parts per million, ppm) and XCH<sub>4</sub> (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO<sub>2</sub> (in ppm) and CH<sub>4</sub> (in ppb).

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<sub>2</sub> and CH<sub>4</sub> 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.



## Executive summary

In this document the retrieval algorithms are described, which are used to generate satellite-derived atmospheric carbon dioxide (CO<sub>2</sub>) and methane (CH<sub>4</sub>) Climate Data Record (CDR) data products as generated via the 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<sub>2</sub> and CH<sub>4</sub>, denoted XCO<sub>2</sub> (in parts per million, ppm) and XCH<sub>4</sub> (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO<sub>2</sub> (in ppm) and CH<sub>4</sub> (in ppb).

These data products are generated from the satellite instruments SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT (XCO<sub>2</sub> and XCH<sub>4</sub> products) and AIRS and IASI (mid/upper tropospheric CO<sub>2</sub> and CH<sub>4</sub> products). All data products are available as Level 2 (individual sounding, i.e., per ground pixels) products in NetCDF format. The XCO<sub>2</sub> and XCH<sub>4</sub> 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<sub>2</sub> and XCH<sub>4</sub> products.

CO<sub>2</sub> and CH<sub>4</sub> 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<sub>2</sub> and CH<sub>4</sub>, 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<sub>2</sub> and CH<sub>4</sub>, 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<sub>2</sub> and 1.8 ppm for CH<sub>4</sub>) 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<sub>2</sub> and CH<sub>4</sub> 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 data set will cover the time period 2003-2016 and is planned to be ready end of October 2017. This data set and its documentation will be made available via the C3S CDS.

The algorithms which are used to retrieve XCO<sub>2</sub> and XCH<sub>4</sub> 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<sub>2</sub> and XCH<sub>4</sub>. These state vector elements are parameters describing the CO<sub>2</sub> and CH<sub>4</sub> 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<sub>2</sub> and XCH<sub>4</sub> 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<sub>2</sub> and CH<sub>4</sub> 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<sub>2</sub> and XCH<sub>4</sub> 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<sub>2</sub> and XCH<sub>4</sub> Level 2 products CO2\_GOS\_SRF and CH4\_GOS\_SRF retrieved using SRON's FP retrieval algorithm
- **ANNEX C:** ATBD for XCH<sub>4</sub> 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<sub>2</sub> and CH<sub>4</sub> 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<sub>2</sub> and CH<sub>4</sub>, denoted XCO<sub>2</sub> (in parts per million, ppm) and XCH<sub>4</sub> (in parts per billion, ppb).
- Mid/upper tropospheric mixing ratios of CO<sub>2</sub> and CH<sub>4</sub>.

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<sub>2</sub> and CH<sub>4</sub> 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<sub>2</sub> and CH<sub>4</sub> (e.g., *Buchwitz et al., 2013a, 2016, 2017*).

These satellite-derived CO<sub>2</sub> and CH<sub>4</sub> 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<sub>2</sub> and CH<sub>4</sub> (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<sub>2</sub> and CH<sub>4</sub> data products is given.



## 1.1 Column-average mixing ratios of CO<sub>2</sub> and CH<sub>4</sub> (XCO<sub>2</sub> and XCH<sub>4</sub>)

### 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<sub>2</sub> and CH<sub>4</sub> 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<sub>2</sub> and CH<sub>4</sub>. The CO<sub>2</sub> and CH<sub>4</sub> products derived from these satellites are column-averaged dry-air mixing ratios (more precisely: mole fractions) of CO<sub>2</sub> and CH<sub>4</sub> denoted XCO<sub>2</sub> (e.g., in ppm) and XCH<sub>4</sub> (e.g., in ppb).

In the following, several satellite instruments are shortly described which are used / can be used to generate XCO<sub>2</sub> and/or XCH<sub>4</sub> 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<sub>2</sub> and XCH<sub>4</sub> 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<sub>2</sub> (e.g., *Reuter et al., 2011; Schneising et al., 2011*) and XCH<sub>4</sub> (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<sub>2</sub> A-band at 760 nm used to obtain the dry-air column using the known 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<sub>2</sub>, CH<sub>4</sub> and O<sub>2</sub> absorption bands in the NIR and SWIR spectral region as needed for accurate XCO<sub>2</sub> and XCH<sub>4</sub> retrieval (in addition GOSAT also covers a large part of the Thermal Infrared (TIR) spectral region). The spectral resolution of TANSO-FTS is 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<sub>2</sub> but not XCH<sub>4</sub>. 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<sub>2</sub> but not XCH<sub>4</sub>. At the time of writing no details on the achieved in-orbit XCO<sub>2</sub> performance of TanSat is available.

### 1.1.2.5 Sentinel-5-Precursor (S5P)

ESA's Sentinel-5-Precursor (S5P) mission (*Veefkind et al., 2012*) is scheduled for launch in mid 2017. S5P will permit XCH<sub>4</sub> retrievals (*Butz et al., 2012*) 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<sub>2</sub> and XCH<sub>4</sub>, the active laser-based mission MERLIN (Methane Remote Sensing Lidar Mission, see [https://de.wikipedia.org/wiki/Merlin\\_\(Satellit\)](https://de.wikipedia.org/wiki/Merlin_(Satellit))) for XCH<sub>4</sub> 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<sub>2</sub> 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<sub>2</sub>

As explained, XCO<sub>2</sub> is the column-averaged dry-air mixing ratio (mole fraction) of atmospheric CO<sub>2</sub>. A XCO<sub>2</sub> value of, for example, 400 ppm at a given location means that about 400 CO<sub>2</sub> molecules are present in the atmosphere above that location per one million air molecules excluding water molecules.

XCO<sub>2</sub> 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<sub>2</sub> ground based observations (e.g., *Dils et al., 2014*).

#### 1.1.4 XCH<sub>4</sub>

As explained, XCH<sub>4</sub> is the column-averaged dry-air mixing ratio (mole fraction) of atmospheric CH<sub>4</sub>. A XCH<sub>4</sub> value of, for example, 1800 ppb at a given location means that about 1800 CH<sub>4</sub> molecules are present in the atmosphere above that location per one billion air molecules excluding water molecules.

XCH<sub>4</sub> 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., 2013*).

These products are validated using Total Carbon Column Observing Network (TCCON) (*Wunch et al., 2010, 2011, 2015*) XCH<sub>4</sub> ground based observations (e.g., *Dils et al., 2014*).



### 1.1.5 List of XCO<sub>2</sub> and XCH<sub>4</sub> data products

Table 2 and Table 3 list the XCO<sub>2</sub> and XCH<sub>4</sub> data products, respectively.

As can be seen from Table 2, for each individual sensor Level 2 XCO<sub>2</sub> 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<sub>2</sub> (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 exist already 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 will be 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 will not be regenerated. They will be provided for C3S « as is » (incl. existing documentation) and made available for the C3S CDS.

Table 2 - Overview XCO<sub>2</sub> 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	Feb. 2017: 2003-2011	Existing GHG-CCI product
CO2_SCI_WFMD	2	SCIAMACHY	Feb. 2017: 2003-2011	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	



As can be seen from Table 3, for each individual sensor Level 2 XCH<sub>4</sub> 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<sub>2</sub> model to correct for XCO<sub>2</sub> variations. FP products contain less data points but the advantage of this product is that it is independent of a CO<sub>2</sub> model.

Table 3 - Overview XCH<sub>4</sub> 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	Feb. 2017: 2003-2011	Existing GHG-CCI product
CH4_SCI_IMAP	2	SCIAMACHY	Feb. 2017: 2003-2011	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<sub>2</sub> and CH<sub>4</sub>

### 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<sub>2</sub> and CH<sub>4</sub> 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<sup>-1</sup> to 2665 cm<sup>-1</sup> (15.4 μm and 3.8 μm), with a spectral resolving power of 1200 (i.e., a spectral resolution ranging from 0.5 cm<sup>-1</sup> to 2 cm<sup>-1</sup>). This domain is divided into three spectral bands, from 650 to 1135 cm<sup>-1</sup>, from 1215 to 1615 cm<sup>-1</sup> and from 2180 to 2665 cm<sup>-1</sup>. 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 in October 2018. IASI provides 8461 spectral samples, ranging from 645 cm<sup>-1</sup> to 2760 cm<sup>-1</sup> (15.5 μm and 3.6 μm), with a spectral sampling of 0.25 cm<sup>-1</sup>, and a spectral resolution of 0.5 cm<sup>-1</sup> 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<sub>2</sub>O), carbon dioxide (CO<sub>2</sub>), carbon monoxide (CO), methane (CH<sub>4</sub>), ozone (O<sub>3</sub>), sulfur dioxide (SO<sub>2</sub>), hydrogen sulfide (H<sub>2</sub>S), ammonia (NH<sub>3</sub>), nitric acid (HNO<sub>3</sub>), 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<sub>2</sub>

Mid-tropospheric columns of CO<sub>2</sub> 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<sub>4</sub>

Mid-tropospheric columns of CH<sub>4</sub> 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<sub>2</sub> and CH<sub>4</sub> data products

Table 4 lists the CO<sub>2</sub> and CH<sub>4</sub> mid/upper troposphere data products.

The product with comment « Existing GHG-CCI product » is the latest versions of AIRS CO<sub>2</sub> 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 will be provided for C3S essentially « as is » (incl. existing documentation) and made available for the C3S CDS. However, it will be converted (from ASCII) to NetCDF format for C3S as will also be done for the IASI products listed in Table 4, i.e., all products listed in Table 4 will be available in NetCDF format.

Table 4 - Overview mid/upper troposphere CO<sub>2</sub> and CH<sub>4</sub> data products.

Product ID	Level	Sensor(s)	(Planned) Availability	Comments
CO2_IASA_NLIS	2	IASI / Metop-A	Oct. 2017: 2007-2015 Oct. 2018: 2007-2017	
CH4_IASA_NLIS	2	IASI / Metop-A	Oct. 2017: 2007-2015 Oct. 2018: 2007-2017	
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	Feb. 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<sub>2</sub> and XCH<sub>4</sub> 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. 9).

## **3. Algorithms for products CO2\_GOS\_SRFP and CH4\_GOS\_SRFP (ANNEX B)**

The products CO2\_GOS\_SRFP and CH4\_GOS\_SRFP are XCO<sub>2</sub> and XCH<sub>4</sub> 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. 9).

## **4. Algorithm for product CH4\_GOS\_SRPR (ANNEX C)**

The product CH4\_GOS\_SRPR is a XCH<sub>4</sub> 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. 9).

## **5. Algorithms for products XCO2\_EMMA and XCH4\_EMMA (ANNEX D)**

The products XCO<sub>2</sub>\_EMMA and XCH<sub>4</sub>\_EMMA are merged multi-sensor XCO<sub>2</sub> and XCH<sub>4</sub> 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. 9).





## 6. Algorithms for CO<sub>2</sub> and CH<sub>4</sub> IASI products (ANNEX E)

The IASI products are mid-tropospheric CO<sub>2</sub> and CH<sub>4</sub> mixing ratios retrieved using algorithms developed at LMD/CNRS, France.

For details see the separate ATBD provided as ANNEX E (see Sect. 9).



## 7. Algorithms for OBS4MIPS XCO<sub>2</sub> and XCH<sub>4</sub> products

The Obs4MIPs XCO<sub>2</sub> and XCH<sub>4</sub> 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<sub>2</sub> and XCH<sub>4</sub> 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<sub>2</sub>) and 12 ppb (XCH<sub>4</sub>) are considered.

In addition to the average XCO<sub>2</sub> and XCH<sub>4</sub> values, also the number of L2 values, the standard deviation of L2 values, and the overall uncertainty  $\sigma$  are computed per L3 grid box. In this context, the overall uncertainty is computed by

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

whereas  $\sigma_m$  represents the standard error of the mean computed from the individual stochastic sounding uncertainties and  $\sigma_i$  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 CO<sub>2</sub>\_SCI\_BESD product

Product: XCO<sub>2</sub>

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 CO<sub>2</sub> 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: CO<sub>2</sub>\_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 XCO<sub>2</sub>; 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](http://www.esa-ghg-cci.org/webfm_send/338)

### 8.2 Algorithm for CO<sub>2</sub>\_SCI\_WFMD and CH<sub>4</sub>\_SCI\_WFMD products

Product: XCO<sub>2</sub> and XCH<sub>4</sub>

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: CO<sub>2</sub>\_SCI\_WFMD & CH<sub>4</sub>\_SCI\_WFMD ATBD:

- Schneising, O., et al., Algorithm Theoretical Basis Document (ATBD) - SCIAMACHY WFM-DOAS (WFMD) XCO<sub>2</sub> and XCH<sub>4</sub> 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](http://www.esa-ghg-cci.org/index.php?q=webfm_send/334)

### 8.3 Algorithm for CH<sub>4</sub>\_SCI\_IMAP product

Product: XCH<sub>4</sub>

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: CH<sub>4</sub>\_SCI\_IMAP ATBD:

- Frankenberg, C., et al., Algorithm Theoretical Basis Document Version 5 (ATBDv5) – The SRON IMAP-DOAS retrieval of XCH<sub>4</sub>, 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](http://www.esa-ghg-cci.org/?q=webfm_send/377)

### 8.4 Algorithm for CO<sub>2</sub>\_AIR\_NLIS product

Product: Mid tropospheric CO<sub>2</sub> 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 CO<sub>2</sub> 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.



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- 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<sub>4</sub>, CO, CO<sub>2</sub>, H<sub>2</sub>O, and N<sub>2</sub>O total column amounts from SCIAMACHY Envisat-1 nadir radiances, *J. Geophys. Res.* 105, 15,231–15,245, 2000.
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## 10. List of ANNEXes

### 10.1 ANNEX A: ATBD for products CO2\_GOS\_OCFP, CH4\_GOS\_OCFP and CH4\_OCPR

Describes algorithms for GOSAT XCO<sub>2</sub> and XCH<sub>4</sub> 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<sub>2</sub> and XCH<sub>4</sub> 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<sub>4</sub> 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<sub>2</sub> and XCH<sub>4</sub> Level 2 products generated by University of Bremen, Germany.

### 10.5 ANNEX E: ATBD for IASI CO<sub>2</sub> and CH<sub>4</sub> products

Describes algorithms for mid-tropospheric CO<sub>2</sub> and CH<sub>4</sub> products from the IASI instrument series generated by LMD/CNRS, France.

*These ANNEXes are available from:*

<https://climate.copernicus.eu/>





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