ESA Climate Change Initiative (CCI)

Product Specification Document (PSD)

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

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Change log:

Version Nr.	Date	Status	Reason for change
Version 1 – Draft 1	14 Dec 2010	Initial Draft for GHG-CCI project team	New document. Main purpose: For distribution to project team for initial input on format of current data products
Version 1 – Draft 2	1st February 2011	Initial Draft for GHG-CCI project team	Updates include common/algorithm-specific sections for ECAs plus input from ULE and SRON on data products.
Version 1 – Draft 3	14th February 2011	Proposed final draft of Version 1	Includes inputs received from project team and feedback from Draft 2
Version 1 - Final	28th February 2011	Final PSDv1	Submitted version
Version 2 – Draft 1	6th March 2012	1st draft of Version 2	New inputs provided by ECA teams
Version 2 - Final	12th March 2012	Final PSDv2	Final comments received from ECA teams - Submitted

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1 Overview

This document is Product Specification Document Version 2 (PSDv2), which is a deliverable of the ESA project GHG-CCI.

The Product Specification Document (PSD) incorporates the user requirements as described in the GHG-CCI User Requirements Document (URD):

URDv1:

Buchwitz, M., F. Chevallier, P. Bergamaschi, I. Aben, H. Bösch, O. Hasekamp, J. Notholt, M. Reuter, et al., User Requirements Document for the GHG-CCI project of ESA's Climate Change Initiative, pp. 45, version 1, 3. February 2011, available from http://www.esa-ghg-cci.org/

The GHG-CCI project will deliver the Essential Climate Variable (ECV) Greenhouse Gases (GHG). Two kinds of algorithms (and their corresponding data products) are used within GHG-CCI:

- ECV Core Algorithms (ECAs): Algorithms to retrieve column-averaged dry air mole fractions of CO_2 and CH_4 from SCIAMACHY/ENVISAT and TANSO/GOSAT, i.e., XCO_2 (in ppm) and XCH_4 (in ppb). These instruments are used as "core instruments" because their measurements are sensitive to the lowest atmospheric layer and therefore provide information on the regional sources and sinks of CO_2 and CH_4.
- Additional Constraints Algorithms (ACAs): Algorithms to retrieve CO_2 and/or CH_4 information on layers above the Planetary Boundary Layer (PBL) such as IASI or MIPAS. They provide additional constrains for inverse modelling of CO_2 and/or CH_4 fluxes by constraining concentrations is upper layers.

For each ECV product the PSD contains the most detailed and specific definition of the:

- geophysical parameters to be provided
- structure and format of the product
- annotation data sets
- quality flags / indicators
- product grid and projection
- ancillary data used

It is recognised that the GHG-CCI project involves a substantial amount of algorithm development and therefore mature data products do not necessarily exist yet. The purpose of this document is to outline the current product specification for each core product with the understanding that this specification is expected to change in the future. These future changes will be reflected in yearly updates to this document.

2 Instruments

This section provides a brief description of the two instruments, SCIAMACHY and GOSAT's TANSO-FTS.

2.1 SCIAMACHY/ENVISAT

The SCanning Imaging Absorption spectroMeter for Atmospheric CartograpHY (SCIAMACHY) is a passive remote sensing spectrometer observing backscattered, reflected, transmitted or emitted radiation from the atmosphere and Earth's surface, in the wavelength range between 240 and 2380 nm. The instrument flies on board ENVISAT which was launched on 1 March 2002. A detailed instrument description is given in **/Bovensmann et al., 1999/**. Until 2009 when GOSAT was launched, SCIAMACHY was the only satellite instrument allowing for the measurement of the atmospheric carbon dioxide and methane concentration with significant sensitivity down to the surface where the sources and sinks are located.

2.2 TANSO/GOSAT

The Japanese Greenhouse gases Observing SATellite (GOSAT) was launched on 23rd January 2009 **/Yokota2009/** by JAXA, the Japanese Space Agency. GOSAT provides the first dedicated global measurements of total column CO_2 and CH_4 from its SWIR bands **/Yoshida2010/**. It is equipped with two instruments, the Thermal And Near Infrared Sensor for carbon Observations - Fourier Transform Spectrometer (TANSO-FTS) as well as a dedicated Cloud and Aerosol Imager (TANSO-CAI).

The TANSO-FTS instrument has four spectral bands with a high spectral resolution 0.3 cm^{-1}, three of which operate in the SWIR at around 0.76, 1.6 and 2.0µm providing sensitivity to the near-surface absorbers with the fourth channel operating in the thermal infrared between 5.5 and 14.3 µm providing mid-tropospheric sensitivity **/Saitoh2009/**.

The measurement strategy of TANSO-FTS is optimised for the characterisation of continental-scale sources and sinks with the aim of achieving a 0.3%-1% relative accuracy for 3-month averages of CO_2 at a 100-1000~km spatial resolution **/Kuze2009/**. The aim for CH_4 is to achieve an accuracy of better than 2% on the same spatial and temporal scales. In order to achieve this, TANSO-FTS utilises a pointing mirror to perform off-nadir measurements at the same location on each 3-day repeat cycle. The pointing mirror allows TANSO-FTS to observe up to ±35° across track and ±20° along-track. These measurements nominally consist of 5 across track points spaced ~100km apart (although measurements are possible with 1, 3, 5, 7 or 9 across track points) with a ground footprint diameter of approximately 10.5 km and a 4 second exposure duration. Whilst the majority of data is limited to measurements over land where the surface reflectance is high, TANSO-FTS also observes in sun-glint mode over the ocean within ±20° of the sub-solar latitude.

3 File format and file naming convention

Data format requirements for GHG-CCI are given in URDv1:

REQ-GHGCCI-DFO-1	The GHG ECV data products shall be in NetCDF format (preferred option) but other data formats are also useful/possible.

Note that the file format and naming conventions are not finalized yet as the GHG-CCI project is currently still in the so-called Round Robin (RR) phase and the algorithms which will be used to generate the first version of the ECV GHG (the so-called Climate Research Data Package (CRDP)) have not yet been selected. The final decision on which algorithms will be used to generate the CRDP will have made end of August 2012. The CRDP will then be generated and will be available in March 2013. The CRDP will be in the final format and the PSDv3, i.e., the next version of this document, will describe that final format. At present, the format is not yet fully defined but current plans are already indicated in this document. Most of the data products are already in the format described in this section. For those data products where this is not the case, the used format is described in a dedicated annex (one per algorithm).

It is planned to use the NetCDF format. Details on the file content are given in the following sections.

Unless otherwise noted, the following common L2 file name convention is foreseen:

The directory structure consists of year (YYYY), month (MM), and day (DD):
/YYYY/MM/DD/

Example: /2010/06/01/

The file names consist of (an abbreviation of) the retrieved gas (GGG), the instrument (III), the algorithm (AAAAAAA), and the orbit's start time (YYYYMMDDHHMMSS):
GGG_III_AAAAAAA_YYYYMMDDHHMMSS.nc

Example: CO2_SCI_WFMD20b_YYYYMMDDHHMMSS.nc

It should be noted that whilst in the development and Round Robin phase, the data will typically be provided as daily or monthly NetCDF files, with the above description becoming relevant when moving to more operational-based processing.

4 ECV Core Algorithms (ECAs)

ECV Core Algorithms (ECAs) are algorithms to retrieve XCO_2 and/or XCH_4 from SCIAMACHY and/or TANSO-FTS. Several ECAs are further developed and assessed within GHG-CCI. At the end of the two year Round Robin time period, the best algorithms to generate one of the four GHG-CCI main data products (XCO_2 and XCH_4 from SCIAMACHY and TANSO-FTS) will be selected. At present at least two different ECAs are used for each of the four main (core) data products.

Table 1 gives a summary of each ECA, including the algorithm identifier and full name, the processing institute, the retrieval technique, relevant references for the retrieval algorithm and the corresponding Appendix, where a detailed product description is given (if available).

ECV Core Algorithm Identifier	Full Name	Institute	Technique	Reference	Appendix For Full Product Description
CO2_SCI_BESD	IUP, Univ. Bremen, Bremen optimal ESimation DOAS (BESD) SCIAMACHY XCO_2 algorithm	IUP	Full Physics, Optimal Estimation	Reuter et al., 2010, 2011	Appendix A
CO2_SCI_WFMD	IUP, Univ. Bremen, Weighting Function Modified DOAS (WFMD) SCIAMACHY XCO_2 algorithm	IUP	Least-squares DOAS (proxy method)	Schneising et al., 2011, 2012	Appendix B
CH4_SCI_WFMD	IUP, Univ. Bremen, Weighting Function Modified DOAS (WFMD) SCIAMACHY XCH_4 algorithm	IUP	Least-squares DOAS (proxy method)	Schneising et al., 2011, 2012	Appendix C
CO2_GOS_OCFP	University of Leicester OCO Full Physics	ULE	Full Physics, Optimal Estimation	Boesch et al., 2006, Connor et al., 2008	Appendix D

	GOSAT CO2				
CH4_GOS_OCFP	University of Leicester OCO Full Physics GOSAT CH4	ULE	Full Physics, Optimal Estimation	Boesch et al., 2006, Connor et al., 2008	Appendix D
CH4_GOS_OCPR	University of Leicester OCO Proxy GOSAT CH4	ULE	Full Physics, Optimal Estimation, 1.6um CH4 and CO2, Proxy	Parker et al., 2011	Appendix D
CH4_SCI_IMAP	SRON Proxy SCIAMACHY CH4	SRON	Proxy method, Iterative maximum a posteriori solution	Frankenberg et al., 2005	Appendix E
CH4_GOS_SRPR	SRON Proxy GOSAT CH4	SRON	Proxy Method, Truncated SVD	Frankenberg et al., 2005	Appendix F
CO2_GOS_SRFP	SRON Full Physics GOSAT CO2	SRON	Full Physics, Phillips-Tikhonov regularization	Butz et al., 2009, 2010	Appendix F
CH4_GOS_SRFP	SRON Full Physics GOSAT CH4	SRON	Full Physics, Phillips-Tikhonov regularization	Butz et al., 2009, 2010	Appendix F

Table 1: Overview ECV Core Algorithms (ECAs).

The data products generated with ECAs contain a common set of parameters (described in the following section) and specific parameters (described in the corresponding Appendix).

4.1 Common Parameters

The users of the GHG ECV data products, as represented by the GHG-CCI CRG, need data products which contain all the information required for surface flux inverse modelling such as retrieved XCO_2 and XCH_4 values for individual ground pixels, their errors, corresponding averaging kernels, a-priori profiles, etc.

In order to provide this and allow comparison during the Round-Robin phase, it is desirable that all ECAs contain the parameters found in the table below where possible.

Dimensions are defined as **number of pixels per orbit (n)** and **number of pressure levels (m).**

Name	Type	Dimensions	Units	Description
instrument	String	1		<SCIAMACHY | GOSAT>
l2_processing_institute	String	1		<IUP | ULE | SRON>
l2_processor_version	String	1		Processor Version Number
l1b_input_filename	String	1		L1B Filename
solar_zenith_angle	Float	n	Degrees	Solar Zenith Angle (0°=zenith)
viewing_zenith_angle	Float	n	Degrees	Viewing Zenith Angle(0°=nadir)
azimuth_difference	Float	n	Degrees	Azimuth Difference
time	Double	n	Seconds	Seconds since 01.01.1970 00:00 UTC
longitude_centre	Float	n	Degrees	Longitude of pixel centre
latitude_centre	Float	n	Degrees	Latitude of pixel centre
longitude_corners	Float	n x 4	Degrees	Longitude of pixel corners (SCIA) or extremes (GOSAT)
latitude_corners	Float	n x 4	Degrees	Latitude of pixel corners (SCIA) or extremes (GOSAT)
surface_elevation	Float	n	km	Mean surface elevation of pixel
pressure_levels	Float	n x m	hPa	Retrieval pressure levels
column_averaging_kernel	Float	n x m		Normalised Column Averaging Kernel Profile
Chi2	Float	n		Chi-Square of fit residual
rms	Float	n		RMS of fit residual
xtarget	Float	n	ppm (CO2) or ppb (CH4)	Retrieved XCO2 (ppm) or XCH4 (ppb)
xtarget_uncertainty	Float	n	ppm (CO2) or ppb (CH4)	Uncertainty in retrieved XCO2 (ppm) or XCH4 (ppb)
xtarget_apriori	Float	n	ppm (CO2) or ppb (CH4)	A priori XCO2 (ppm) or XCH4 (ppb)
vmr_profile_target	Float	n x m	ppm (CO2) or ppb (CH4)	Retrieved XCO2 (ppm) or XCH4 (ppb) profile
vmr_profile_target_uncertainty	Float	n x m	ppm (CO2) or ppb (CH4)	Uncertainty in retrieved XCO2 (ppm) or XCH4 (ppb) profile
vmr_profile_target_apriori	Float	n x m	ppm (CO2) or ppb (CH4)	A priori XCO2 (ppm) or XCH4 (ppb) profile

Table 2: Common parameters for the SCIAMACHY and TANSO XCO_2 and XCH_4 data products generated with ECAs.

4.2 Algorithm-Specific Parameters

In addition to the common parameters listed above, a full description of all algorithm-specific parameters is provided in the Appendices to this document. Please see **Table 2** for the corresponding Appendix.

5 Additional Constraints Algorithms (ACAs)

A short description of the additional constraints algorithms (ACAs) are provided in Appendix G.

The Additional Constraints Algorithms, listed by institute are:

Laboratoire de Météorologie Dynamique (LMD)

- CO2_AIR_NLIS – AIRS CO_2
- CO2_IAS_NLIS – IASI CO_2
- CH4_IAS_NLIS – IASI CH_4
- CO2_ACE_CLSR – ACE-FTS CO_2

Karlsruhe Institute of Technology (KIT)

- CH4_MIP_IMK – MIPAS CH_4

Institute of Environmental Physics (IUP)

- CH4_SCI_ONPD – SCIAMACHY Solar Occultation CH_4

6 References

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7 Terms and Acronyms

Terms

The terms listed below have been defined in **/CMUG-RBD, 2010/** and are repeated here as this document shall be consistent with **/CMUG-RBD, 2010/**. In case a different meaning is used in this document this is mentioned in this document.

Term	Meaning
Data assimilation	Observations directly influence the model initial state taking into account their error characteristics during every cycle of a model. This is used for reanalysis and NWP.
Model validation	Observations are compared with equivalent model fields to assess the accuracy of the model. This can be on short time scales for process studies or long time scales for climate trends.
Climate monitoring	This describes the use of a satellite only dataset to monitor a particular atmospheric or surface variable over a period > 15yrs to investigate whether there is a trend due to climate change.
Initialisation	To initialise prognostic quantities of the model with reasonable values at the beginning of the simulation but do not continuously update.
Prescribe boundary conditions	Prescribe boundary conditions for a model run for variable that are not prognostic (e.g. land cover, ice caps etc).

Acronyms

Abbreviation	Meaning
ACE-FTS	Atmospheric Chemistry Experiment-Fourier Transform Spectrometer (ASC/SCISAT-1)
AAI	Absorbing Aerosol Index
AATSR	Advanced Along Track Scanning Radiometer
AIRS	Atmospheric Infrared Sounder
AMSU	Advanced Microwave Sounding Unit
AOD	Aerosol Optical Depth
AOT	Aerosol Optical Thickness
ATBD	Algorithm Theoretical Basis Document
BESD	Bremen optimal EStimation DOAS
CCI	Climate Change Initiative
COD	Cloud Optical Depth
COTS	Commercial Off-The-Shelf software
D/B	Data base
DOAS	Differential Optical Absorption Spectroscopy
DPM	Detailed Processing Model
EC	European Commission
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EO	Earth Observation
ESA	European Space Agency
ESM	Earth System Model
FCDR	Fundamental Climate Data Record
FP	Full Physics

FSI-WFM-DOAS	Full Spectral Initiasation WFM-DOAS
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 Gas Observing Satellite
GTOS	Global Terrestrial Observing System
IASI	Infrared Atmospheric Sounding Interferometer
IDL	Interactive Data Language
ITT	Invitation To Tender
IMAP-DOAS	Iterative Maximum A posteriori DOAS
IMLM	Iterative Maximum Likelihood Method
IODD	Input Output Data Definition
IPCC	International Panel in Climate Change
IPR	Intellectual Property Right
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
KO	Kick-Off Meeting
LMD	Laboratoire de Météorologie Dynamique
LUT	Look-up table
MACC	Monitoring Atmospheric Composition and Climate, EU GMES project
MERIS	Medium Resolution Imaging Spectrometer
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
MODIS	Moderate Resolution Imaging Spectrometer
MRT	Mid-term Review

NA	Not applicable
NDACC	Network for the Detection of Atmospheric Composition Change
NASA	National Aeronautics and Space Administration
NIES	National Institue for Environmental Studies
NOAA	National Oceanic and Atmospheric Administration
OCO	Orbiting Carbon Observatory
OD	Optical Depth
OE	Optimal Estimation
PBL	Planetary Boundary Layer
PM	Progress Meeting
PMD	Polarization Measurement Device
PMP	Project Management Plan
PVP	Product Validation Plan
PVR	Product Validation Report
RD	Reference Document
RTM	Radiative transfer model
SCIATRAN	Radiative transfer model for SCIAMACHY developed and continuously improved at IUP
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY
SoW	Statement of work
SQWG	SCIAMACHY Quality Working Group
SRD	Software Requirements Document
SUM	Software User Manual
SVR	Software Verification Report
TANSO	Thermal And Near infrared Sensor for carbon Observation
TBC	To be confirmed
TCCON	Total Carbon Column Observing Network
TBD	To be defined / to be determined

TES	Tropospheric Emission Spectrometer
TOVS	TIROS Observationnal Vertical Sounde
WFM-DOAS (or WFMD)	Weighting Function Modified DOAS

8 Appendix A - CO2_SCI_BESD

The Bremen Optimal Estimation DOAS (BESD) algorithm **/Reuter et al., 2010, 2011/** is IUP's full physics XCO_2 retrieval. It aims to significantly reduce scattering related errors of SCIAMACHY retrieved XCO_2. It uses SCIAMACHY nadir data at 0.76 and 1.6 µm and explicitly considers scattering by an (optically thin) ice cloud layer and aerosols assuming a default profile. The scattering information is transferred from the O_2-A band to the CO_2 band by using a merged fit window approach to simultaneously retrieve scattering related parameters and XCO_2.

8.1 Data organization

The data organization follows the common definitions given in this document for all ECV core algorithms with the difference that one file per day (but not per orbit) is produced. All retrievals of a single day which pass initial quality checks are packed into an individual NetCDF file.

8.1.1 File naming convention

Adapted from Section 3.
(CO2_SCI_BESD_vXX.XX.XX_YYYYMMDD.nc)

8.1.2 Common data fields

As commonly defined within this document (see Section 4.1).

8.1.3 Algorithm specific data fields

The following table describes the planned additional contents of the final ECV data product (i.e., parameters which will be provided in addition to the common parameters). Type, dimension, units and description will be specified after implementation. Essentially, it describes the fields of the current, internal file format. Therefore, this list is preliminary and may change during the project if adaptations are needed.

Name	Type	Dimensions	Units	Description
ORBIT_NR	tbs	tbs	tbs	tbs
CALIBR_APPL	tbs	tbs	tbs	tbs
WAVELENGTH_NADIR	tbs	tbs	tbs	tbs
RADIANCE_NADIR	tbs	tbs	tbs	tbs
ERROR_NADIR	tbs	tbs	tbs	tbs
WAVELENGTH_SOLAR	tbs	tbs	tbs	tbs
RADIANCE_SOLAR	tbs	tbs	tbs	tbs
ERROR_SOLAR	tbs	tbs	tbs	tbs

ECMWF_HEIGHT	tbs	tbs	tbs	tbs
ECMWF_TEMPERATURE	tbs	tbs	tbs	tbs
ECMWF_PRESSURE	tbs	tbs	tbs	tbs
ECMWF_H2O	tbs	tbs	tbs	tbs
GTOPO30_HEIGHT	tbs	tbs	tbs	tbs
GTOPO30_ROUGH	tbs	tbs	tbs	tbs
LAND_SEA_FRACTION	tbs	tbs	tbs	tbs
MERIS_CFC	tbs	tbs	tbs	tbs
SCIAMACHY_AAI	tbs	tbs	tbs	tbs
A_PRIORI_ERROR_COVARIANCE_MATRIX	tbs	tbs	tbs	tbs
STATE_VECTOR_NAMES	tbs	tbs	tbs	tbs
STATE_VECTOR_A_PRIORI	tbs	tbs	tbs	tbs
STATE_VECTOR_A_PRIORI_ERROR	tbs	tbs	tbs	tbs
STATE_VECTOR_RETRIEVED	tbs	tbs	tbs	tbs
STATE_VECTOR_RETRIEVED_ERROR	tbs	tbs	tbs	tbs
STATE_VECTOR_REFERENCE	tbs	tbs	tbs	tbs
STATE_VECTOR_FIT_WINDOW	tbs	tbs	tbs	tbs
INTENSITY_FIT	tbs	tbs	tbs	tbs
WAVELENGTH_FIT	tbs	tbs	tbs	tbs
INTENSITY_MEASUREMENT	tbs	tbs	tbs	tbs
INTENSITY_REFERENCE	tbs	tbs	tbs	tbs
WAVELENGTH_REFERENCE	tbs	tbs	tbs	tbs
INTENSITY_RMSE	tbs	tbs	tbs	tbs
INTENSITY_CHI2	tbs	tbs	tbs	tbs
NUMBER_OF_ITERATIONS	tbs	tbs	tbs	tbs
CONVERGENCE	tbs	tbs	tbs	tbs
JACOBIAN_FIT	tbs	tbs	tbs	tbs
NUMBER_OF_FIT_WINDOWS	tbs	tbs	tbs	tbs
SIZE_OF_FIT_WINDOWS	tbs	tbs	tbs	tbs
MEASUREMENT_ERROR_COVARIANCE_MATRIX	tbs	tbs	tbs	tbs
GAIN_MATRIX	tbs	tbs	tbs	tbs
AVERAGING_KERNEL_MATRIX	tbs	tbs	tbs	tbs
DEGREE_OF_FREEDOM	tbs	tbs	tbs	tbs
R_MATRIX	tbs	tbs	tbs	tbs
INFORMATION_CONTENT	tbs	tbs	tbs	tbs
ERROR_COVARIANCE_SMOOTHING	tbs	tbs	tbs	tbs
ERROR_COVARIANCE_NOISE	tbs	tbs	tbs	tbs
ERROR_COVARIANCE_STATISTICAL	tbs	tbs	tbs	tbs
STATE_VECTOR_ERROR_REDUCTION	tbs	tbs	tbs	tbs
STATE_VECTOR_INFORMATION_CONTENT	tbs	tbs	tbs	tbs
STATE_VECTOR_DEGREE_OF_FREEDOM	tbs	tbs	tbs	tbs
XCO2_ERROR_SMOOTHING	tbs	tbs	tbs	tbs
XCO2_ERROR_NOISE	tbs	tbs	tbs	tbs
XCO2_ERROR_REDUCTION	tbs	tbs	tbs	tbs
XCO2_DEGREE_OF_FREEDOM	tbs	tbs	tbs	tbs
XCO2_INFORMATION_CONTENT	tbs	tbs	tbs	tbs

Table 3: Additional parameters of the data product generated with the CO2_SCI_BESD algorithm. tbs = to be specified.

9 Appendix B - CO2_SCI_WFMD

The Weighting Function Modified Differential Optical Absorption Spectroscopy (WFM-DOAS) retrieval technique was developed for the retrieval of trace gases and optimised for CO_2, CH_4, and O_2 retrievals using a fast look-up table (LUT) scheme to avoid computationally expensive online radiative transfer calculations. The current version is WFMDv2.2, which is a further development of WFMDv2.1 described in **/Schneising et. al, 2011,2012/**.

In order to convert the retrieved CO_2 columns into column-averaged mole fractions the CO_2 columns are divided by the dry-air columns obtained from the simultaneously measured O_2 columns obtained from the O_2 A-band.

9.1 Data organization

All retrievals of a given month passing the quality filter are integrated in a single ASCII-file.

9.1.1 File naming convention

SCI_WFMD_L2_w6002_yyyymm_v2.2.was

9.1.2 Data Contents

This list of data fields may be subject to changes during the project.

```
px#           : Ground pixel number (per orbit) [-] (1,2,...)
st#           : State number [-] (0,1,..)
read#         : Ground pixel number (per state) [-] (0,1,...)
t             : Pixel type [-] (1:forward 2:backscan)
dsr_time      : Starttime in fractional days since 1.1.2000 [day] (0.x=1.1.2000)
t_int         : Integration time [s]
lat_c         : Latitude  center   [deg]
lon_c         : Longitude center   [deg]
lat_1         : Latitude  corner 1 [deg]
lon_1         : Longitude corner 1 [deg]
lat_2         : Latitude  corner 2 [deg]
lon_2         : Longitude corner 2 [deg]
lat_3         : Latitude  corner 3 [deg]
lon_3         : Longitude corner 3 [deg]
lat_4         : Latitude  corner 4 [deg]
lon_4         : Longitude corner 4 [deg]
sza           : Solar zenith angle [deg]
los           : Line-of-sight zenith angle [deg]
azi           : Relative azimuth angle [deg]
cld           : PMD cloud mask (1:probably cloud contaminated)
lnd           : Land mask (1:completely land covered)
snrad         : Sun-normalized radiance (R/I*PI) at 1560 nm [-]
alt           : Average ground altitude [km]
H2O(CO2 fit)  : H2O column of CO2 fit [molec./cm2]
H2O_err(CO2)  : H2O column error of CO2 fit [%]
H2O_VCA       : H2O vertical column amount [g/cm2]
H2O_REF_INT   : Reference averaged sun-normalized radiance (1395.0 - 1410.0 nm)
H2O_INT       : Averaged sun-normalized radiance (1395.0 - 1410.0 nm)
H2O_PARA      : (H2O_INT / H2O_REF_INT) - 1
O2#           : Number of O2 (sub-)pixel [-]
ALB760        : ALBEDO @ 756nm
O2            : O2 column [molec./cm2]
O2_err        : O2 column error [%]
O2_rms        : RMS of O2 fit residuum [-]
O2Q           : O2 quality flag (0:good 1:bad)
O2_REF        : Reference O2 column (from surface elevation)
O2_CRIT       : O2 / O2_REF
O2_CRIT_LOS   : O2_CRIT scan-angle-bias corrected
CO2#          : Number of CO2 (sub-)pixel [-]
ALB1560       : ALBEDO @ 1559nm
CO2           : CO2 column [molec./cm2]
CO2_err       : CO2 column error [%]
CO2_rms       : RMS of CO2 fit residuum [-]
CO2Q          : CO2 quality flag (0:good 1:bad)
XCO2          : XCO2 [ppm]
XCO2_err      : XCO2 error [%]
XCO2Q         : XCO2 quality flag (0:good 1:bad)
XCO2_LOS      : XCO2 scan-angle-bias corrected [ppm]
XCO2_WFMDv22  : XCO2 final product [ppm]
XCO2FQ        : XCO2 final quality flag (0:good 1:bad)
```

9.1.3 Data Usage

Note that column counting in product files starts at 0.
Please use XCO2_WFMDv22 (Column 48) of *.was with the following filter criteria:
XCO2FQ = 0 (Column 49)

10 Appendix C - CH4_SCI_WFMD

The current version is WFMDv2.3, which is a further development of WFMDv2.0.2 described in **/Schneising et. al, 2011,2012/**.

In order to convert the retrieved CH_4 columns into column-averaged mole fractions the CH_4 columns are divided by the dry-air columns obtained from the simultaneously measured CO_2 columns correcting for CO_2 variability using CarbonTracker.

10.1 Data organization

All retrievals of a given month passing the quality filter are integrated in a single ASCII-file.

10.1.1 File naming convention

SCI_WFMD_L2_w6002_yyyymm_v2.3.was

10.1.2 Data Contents

This list of data fields may be subject to changes during the project.

```
px#           : Ground pixel number (per orbit) [-] (1,2,...)
st#           : State number [-] (0,1,..)
read#         : Ground pixel number (per state) [-] (0,1,...)
t             : Pixel type [-] (1:forward 2:backscan)
dsr_time      : Starttime in fractional days since 1.1.2000 [day] (0.x=1.1.2000)
t_int         : Integration time [s]
lat_c         : Latitude  center   [deg]
lon_c         : Longitude center   [deg]
lat_1         : Latitude  corner 1 [deg]
lon_1         : Longitude corner 1 [deg]
lat_2         : Latitude  corner 2 [deg]
lon_2         : Longitude corner 2 [deg]
lat_3         : Latitude  corner 3 [deg]
lon_3         : Longitude corner 3 [deg]
lat_4         : Latitude  corner 4 [deg]
lon_4         : Longitude corner 4 [deg]
sza           : Solar zenith angle [deg]
los           : Line-of-sight zenith angle [deg]
azi           : Relative azimuth angle [deg]
cld           : PMD cloud mask (1:probably cloud contaminated)
lnd           : Land mask (1:completely land covered)
snrad         : Sun-normalized radiance (R/I*PI) at 1560 nm [-]
alt           : Average ground altitude [km]
H2O(CH4 fit)  : H2O column (CH4 window) [g/cm2]
H2O_err(CH4)  : H2O column error (CH4 window) [%]
H2O(CO2 fit)  : H2O column (CO2 window) [g/cm2]
H2O_err(CO2)  : H2O column error (CO2 window) [%]
O2#           : Number of O2 (sub-)pixel [-]
O2            : O2 column [molec./cm2]
O2_err        : O2 column error [%]
O2_rms        : RMS of O2 fit residuum [-]
O2Q           : O2 quality flag (0:good 1:bad)
CO2#          : Number of CO2 (sub-)pixel [-]
CO2           : CO2 column [molec./cm2]
CO2_err       : CO2 column error [%]
CO2_rms       : RMS of CO2 fit residuum [-]
CO2Q          : CO2 quality flag (0:good 1:bad)
CH4           : CH4 column [molec./cm2]
CH4_err       : CH4 column error [%]
CH4_rms       : RMS of CH4 fit residuum [-]
CH4Q          : CH4 quality flag (0:good 1:bad)
XCH4_v2.0.2   : XCH4 WFMDv2.0.2 [ppb]
XCH4_err      : XCH4 error [%]
XCH4_v2.3     : XCH4 WFMDv2.3 [ppb]
XCH4FQ        : XCH4 final quality flag (0:good 1:bad)
```

10.1.3 Data Usage

Note that column counting in product files starts at 0.
Please use XCH4_v2.3 (Column 43) of *.was with the following filter criteria:
XCH4FQ = 0 (Column 44)

11 Appendix D - CO2_GOS_OCFP, CH4_GOS_OCFP and CH4_GOS_OCPR

This section provides the full product description for the CO2_GOS_OCFP, CH4_GOS_OCFP and CH4_GOS_OCPR data products processed at the University of Leicester.

The OCO `full physics' retrieval algorithm was developed for the NASA Orbiting Carbon Observatory (OCO) mission (now the Atmospheric Carbon Observations from Space (ACOS) project) to retrieve XCO_2 (dry air, column averaged, mole fraction of CO_2) from a simultaneous fit of SWIR O_2 and CO_2 bands. For a detailed description please see **/Boesch et al., 2006/**,**/Boesch et al., 2010/** and **/Connor et al., 2008/.**

The retrieval algorithm performs an iterative retrieval based on the optimal estimation approach **/Rodgers, 2000/** to estimate a set of atmospheric/surface/instrument parameters (i.e. the state vector, **x**) from the measured spectral radiances **/Connor et al., 08/**. The version of the OCO algorithm used here utilises the LIDORT radiative transfer model to relate the state vector to the observed radiances, incorporating a fast 2-orders-of-scattering vector radiative transfer code **/Natraj et al., 2008/**. We also use the low-streams interpolation functionality of the code **/O'Dell et al., 2010/** in order to accelerate the radiative transfer component of the retrieval algorithm.

The state vector typically consists of profiles for CO_2, CH_4, H_2O, temperature and aerosol extinction along with surface pressure, surface albedo and a spectral shift/stretch. In order to reduce the number of elements in the state vector, we replace the full profiles for H_2O and temperature with a profile scaling factor. The final XCO_2 is computed from the retrieved state after the iterative retrieval has converged.

11.1 Data organisation

All retrievals for a single month (or TCCON site) are packaged into a single NetCDF file. A quality flag is included which **must** be applied to the data in order to select the retrievals which have passed our post-processing quality control.

11.2 File naming convention

The GOSAT L1B naming convention is as follows:
GOSATTFTS_yyyymmddhhMMPPPSSSX_1BTTTTVVVVVV
Table 4 describes this in full and provides an example based on the following GOSAT L1B data file:
GOSATTFTS2010053107470120300_1BOB1D100100

Symbol	Name	Example
yyyy	Year	2010
mm	Month	05
dd	Day	31
HH	Hour	07
MM	Minute	47
PPP	Path/Orbit Number	012 (range 001 to 044)
SSS	Scene Number	030 (range 001 to 060)
X	Sub-scene Number	0
TTTT	Observation Type	OB1D
VVVVVV	L1B Version Number	100100

Table 4: Description of GOSAT L1B file naming conventions

It is planned that the final retrieved data product adopts a similar naming convention but as a consequence of all retrievals for a single path/orbit being combined the name format is:

CO2_GOS_OCFP<processor_version>_yyyymmddhhMMPPP
CH4_GOS_OCFP<processor_version>_yyyymmddhhMMPPP
CH4_GOS_OCPR<processor_version>_yyyymmddhhMMPPP

Note that for the Round Robin phase of the GHG CCI process, the data are instead packaged into single monthly netcdf files.

11.3 Data Contents

The following table describes in full the contents of the final CO2_GOS_OCFP and CH4_GOS_OCFP data products with variable name, type, dimension, units and description.

Name	Type	Dimensions	Units	Description
numexp		1		Number of exposures
num_levels		1		Number of levels
exp_id	byte	22 x numexp		Exposure ID
year	Float	numexp		Year
month	Float	numexp		Month
day	Float	numexp		Day
hour	Float	numexp		Hour
min	Float	numexp		Min
sec	Float	numexp		Sec
lat	Float	numexp	degrees	Latitude
lon	Float	numexp	degrees	Longitude
sza	Float	numexp	degrees	Solar Zenith Angle
surface_alt	Float	numexp	metres	Surface Altitude
surface_alt_std	Float	numexp	metres	Surface Altitude Standard Deviation in Footprint
ap_psurf	Float	numexp	Pa	Apirori Surface Pressure
ap_psurf_std	Float	numexp	Pa	Apirori Surface Pressure Standard Deviation in Footprint
quality_flag	Float	numexp		Quality Flag (1=good, 0=bad)
gain	Float	numexp		Instrument Gain Mode
xco2 | xch4	Float	numexp	ppm	XCO2 | XCH4
xco2_error | xch4_error	Float	numexp	ppm	XCO2 Error | XCH4 Error
xco2_bias_corrected	Float	numexp	ppm	XCO2 with preliminary bias correction applied (Note: not currently available for XCH4)
outcome	Float	numexp		Retrieval Outcome
pressure	Float	num_levels x numexp	Pa	Pressure Retrieval Grid
apriori_temperature	Float	num_levels x numexp	K	A Priori Temperature Profile
apriori_h2o	Float	num_levels x numexp		A Priori H2O Profile
apriori_ch4	Float	num_levels x numexp		A Priori CH4 Profile
apriori_co2	Float	num_levels x numexp		A Priori CO2 Profile
ch4_averaging_kernel	Float	num_levels x numexp		CH4 Averaging Kernel
co2_averaging_kernel	Float	num_levels x numexp		CO2 Averaging Kernel
a_aod	Float	numexp		A Priori Aerosol Optical Depth
a_aod_1	Float	numexp		A Priori AOD Profile 1
a_aod_2	Float	numexp		A Priori AOD Profile 2
a_aod_4	Float	numexp		A Priori AOD Profile 4 (ice)
r_aod	Float	numexp		Retrieved Aerosol Optical Depth
r_aod_1	Float	numexp		Retrieved AOD Profile 1
r_aod_2	Float	numexp		Retrieved AOD Profile 2
r_aod_4	Float	numexp		Retrieved AOD Profile 4 (ice)

Table 5: Additional parameters of the data product generated with the CO2_GOS_OCFP and CH4_GOS_OCFP algorithms.

Name	Type	Dimensions	Units	Description
numexp		1		Number of exposures
num_levels		1		Number of levels
exp_id	byte	22 x numexp		Exposure ID
year	Float	numexp		Year
month	Float	numexp		Month
day	Float	numexp		Day
hour	Float	numexp		Hour
min	Float	numexp		Min
sec	Float	numexp		Sec
lat	Float	numexp	degrees	Latitude
lon	Float	numexp	degrees	Longitude
sza	Float	numexp	degrees	Solar Zenith Angle
surface_alt	Float	numexp	metres	Surface Altitude
surface_alt_std	Float	numexp	metres	Surface Altitude Standard Deviation in Footprint
ap_psurf	Float	numexp	Pa	Apirori Surface Pressure
ap_psurf_std	Float	numexp	Pa	Apirori Surface Pressure Standard Deviation in Footprint
quality_flag	Float	numexp		Quality Flag (1=good, 0=bad)
gain	Float	numexp		Instrument Gain Mode
xco2	Float	numexp	ppm	Retrieved 1.6um XCO2
xco2_error	Float	numexp	ppm	Retrieved 1.6um XCO2 Error
xch4	Float	numexp	ppb	Retrieved 1.6um XCH4
xch4_error	Float	numexp	ppb	Retrieved 1.6um XCH4 Error
proxy_xch4	Float	numexp	ppb	Proxy XCH4
proxy_xch4_error	Float	numexp	ppb	Proxy XCH4 Error
outcome	Float	numexp		Retrieval Outcome
pressure	Float	num_levels x numexp	Pa	Pressure Retrieval Grid
apriori_temperature	Float	num_levels x numexp	K	A Priori Temperature Profile
apriori_h2o	Float	num_levels x numexp		A Priori H2O Profile
apriori_ch4	Float	num_levels x numexp		A Priori CH4 Profile
apriori_co2	Float	num_levels x numexp		A Priori CO2 Profile
ch4_averaging_kernel	Float	num_levels x numexp		CH4 Averaging Kernel
co2_averaging_kernel	Float	num_levels x numexp		CO2 Averaging Kernel
a_aod	Float	numexp		A Priori Aerosol Optical Depth

Table 6: Parameters of the data product generated with the CH4_GOS_OCPR algorithm.

12 Appendix E - CH4_SCI_IMAP

This section provides the full product description for the CH4_SCI_IMAP data product processed at SRON.

12.1 Data organisation

All converging retrievals for a single orbit are saved in a single netCDF4 file.

12.2 File naming convention

The SCIAMACHY L1B file names include the sequence

- product ID: SCI_NL__0P, SCI_NL__ 1P or SCI_NL__ 2P for level 0, 1b or 2 data
- processing status flag: N for NRT products, letters between N and V for consolidated products
- originator ID: PDK, PDE, LRA, D-P for PDHS-K, PDHS-E, LRAC or D-PAC
- start date: year, month and day of measurement start
- start time: hours, minutes and seconds of measurement start in UTC
- duration of product coverage in seconds
- ENVISAT mission phase
- ENVISAT cycle number
- relative orbit number within cycle
- absolute orbit number at product start
- file counter
- file extension: N1 corresponds to ENVISAT

An example for a L1 filename is:
SCI_NL__1PUDPA20100101_002615_000060322085_00346_40981_1171.N1
We maintain most of the naming convention for our HDF5 L2 XCH_4 files. The L2 file corresponding to the previous L1B file would be:
SCI_IMAP_1PUDPA20100101_002615_000060322085_00346_40981_1171_small.nc

12.3 Data Contents

The following table details the content of each netCDF4 file (containing n retrievals).

Name	Type	Dimensions	Units	Description
/OrbitGeometry				
center_atitude	Float	n	degrees	Geodetic latitude of pixel centre
center_longitude	Float	n	degrees	Geodetic longitude of pixel centre
line_of_sight_zenith	Float	n	degrees	Line of sight zenith angle
solar_zenith	Float	n	degress	Solar zenith angle
solar_azimuth	Float	n	degress	Solar Azimuth angle
satellite_azimuth	float	n	Degrees	viewing azimuth angle
Integration_time	Float	n	seconds	Integration time
corner_latitudes	Float	(n,4)	degrees	Latitude of the 4 corners of the ground-pixel
corner_longitudes	Float	(n,4)	degrees	Longitude of the 4 corners of the ground-pixel
surface_altitude	Float	n	meter	Ground pixel surface elevation
AirMassFactor	Float	n	Modified julian day	Sounding time
orbitalPhase	Float	n		orbital phase (from L1B file)
scan_range	Float	n	Degree	Absolute range of line of sight zenith angles
pet	Float	n	seconds	Pixel Exposure Time
dry_air_column_ecmwf	Float	n	Molec/cm^2	Dry air column derived from ECMWF
h2o_air_column_emcwf	Float	N	Molec/cm^2	H_2O air column derived from ECMWF
time_mjd	Double	n		Modified Julian Day
surface_pressure	Float	n	hPa	Surface Pressure
/HighLevelResults/ch4_v60_esa_1pix				
ch4_vcd	Float	n	molec/cm^2	Methane vertical column density
ch4_vcd_sigma	Float	n	molec/cm^2	1-sigma precision error in methane vertical column density
co2_vcd	Float	n	molec/cm^2	Carbon dioxide vertical column density
co2_vcd_sigma	Float	n	molec/cm^2	1-sigma precision error in CO_2 vertical column density
xCH4_retrieved	Float	n	ppb	Derived column averaged dry methane mixing ratio
xCH4_1sigma	Float	n	ppb	1-sigma precision error in xVMR_CH4
xCH4_prior	Float	N	ppb	Prior XCH_4 from TM4
co2_column_averaging_kernel	Float	n x m	-	CO_2 total column averaging kernel for 10 layers per sounding
ch4_column_averaging_kernel	Float	n x m	-	CH_4 total column averaging kernel for 10 layers per sounding
layer_ch4_prior_vcd	Float	n x m	Molec/cm^2	CO_2 prior VCD profile (10

				layers)
layer_co2_prior_vcd	Float	n x m	Molec/cm^2	CH_4 prior VCD profile (10 layers)
layer_dry_air_vcd	Float	n x m	Molec/cm^2	Dry air VCD per layer (10 layers, to derive VMRs from prior trace gas VCDs)
layer_lower_level	Float	n x m	hPa	Lower pressure levels of m retrieval layers
layer_upper_level	Float	n x m	hPa	Upper pressure levels of m retrieval layers
QualityFlag	Float	n	-	Quality flag or retrieval - 1=failed, 0=converged but probably cloudy, 1=converged and supposedly cloud free
MaxErrorDarkCurrent	Float	n	BU	Maximum absolute readout of Q-branch detector pixel at SZAs>95 degrees
MaxQBranchResidual	Float	n	radiance	Maximum absolute residuum in the Q-branch
MaxQBranchResidual_weighted	Float	n	radiance	Maximum weighted (by noise) residuum in the Q-branch
VCD_CO2_MODEL	Float	n	molec/cm^2	model CO2 vertical column density used to derive xCH_4
/RetrievalResults				
ch4_v60_esa_1pix/SpectralParameters/residual_rms	Float	n	-	fit residual RMS for the CH_4 fit window
ch4_v60_esa_1pix/SpectralParameters/residual_reduced_chi2	Float	n	-	fit reduced chi^2 for the CH_4 fit window
co2_v60_v1/SpectralParameters/residual_rms	Float	n	-	fit residual RMS for the CO_2 fit window
co2_v60_v1/SpectralParameters/residual_reduced_chi2	Float	n	-	fit reduced chi^2 for the CO_2 fit window
ch4_v60_esa_1pix/Ancillary/iterations	Float	n	-	number of iterations used in the CH_4 fit
co2_v60_v1/Ancillary/iterations	Float	n	-	number of iterations used in the CO_2 fit

Table 7: Additional parameters of the data product generated with the CH4_SCI_IMAP algorithm.

13 Appendix F - CO2_GOS_SRFP, CH4_GOS_SRFP and CH4_GOS_SRPR

This section provides the full product description for the GOSAT data products processed at SRON.

Using the Full Physics method, we retrieve simultaneously XCH_4 and XCO_2, as well as three aerosol parameters representing their amount, height distribution and size distribution. For this study, we analyse four spectral regions: the 0.77 µm oxygen band, two CO_2 bands at 1.61 and 2.06 µm, as well as a CH_4 band at 1.64 µm.

Data products are obtained from spectra that pass several quality requirements: no GOSAT error flags, SZA < 70 degrees, SNR > 50. Cloudy scenes are removed beforehand using CAI level 2 products.
All retrievals for each month will be saved in a single NetCDF file.

Table 8 describes the contents of the full physics data products (name, type, dimension, units and description of variables).

Using the proxy method, we retrieve simultaneously XCH_4 and XCO_2 in clear sky conditions (no scattering from aerosols nor rayleigh scattering). Only the CO_2 band and the CH_4 band around 1.6 µm are used. We then take the ratio XCH_4/XCO_2 and multiply it by the a priori XCO_2 (which comes from CarbonTracker, including a correction for 2010 and 2011 values).

Data product from this proxy method is the same as for the full physics method except that as we do not include scattering, the quantities DFS for aerosols and retrieved optical thickness are irrelevant and not provided. We additionally provide the quantities APR_XCO2_CORR, XCH4_proxy=XCH4/XCO2 *APR_XCO2_corr and XCH4_proxy_uncertainty.

Name	Type	Dim.	Units	Description
n	Integer	1		Number of exposures in file
Instrument	String	1		'GOSAT'
L2_processing_Institute	String	1		'SRON'
L2_processor_version	String	1		'RemoteC_x.x'
GOSAT_filename	String	n		GOSAT filenames, format yyyymmddhhMMPPPSSSXIdexpo (see table in section Appendix A)
gosat_obsmode	String	n		Observation mode: 'OB1D', 'OB1N', 'OB2D', 'SPOD', 'SPON', 'CALM', 'LUCA'
gosat_gain	String	n		Observation gain:'HH','MM'
gosat_flag_sunglint	Integer	n		0 = Nadir, 1 = Glint
gosat_flag_landtype	Integer	n		0 = Land, 1 = Ocean
gosat_error_flags	Integer	n,9		9 GOSAT error flags
GOSAT_Date	Integer	n,5		Year, Month, Day, Hour, Minute
GOSAT_Seconds	Float	n		Second
GOSAT_Latitude_centre	Float	n	degrees	Centre Latitude
GOSAT_Longitude_centre	Float	n	degrees	Centre Longitude
GOSAT_Latitude_corners	Float	n,4	degrees	Latitude extremes in GOSAT FOV
GOSAT_Longitude_corners	Float	n,4	degrees	Longitude extremes in GOSAT FOV
GOSAT_Solar_Zenith_Angle	Float	n	degrees	Solar Zenith angle
GOSAT_Solar_Azimuth_Angle	Float	n	degrees	Solar Azimuth angle
GOSAT_Viewing_Zenith_Angle	Float	n	degrees	Satellite Zenith angle
GOSAT_Viewing_Azimuth_Angle	Float	n	degrees	Satellite azimuth angle
gosat_IFOV_Cloud_flags_nyes	Integer	n		Number of CAI valid pixels that match GOSAT footprint
gosat_IFOV_Cloud_flags_nno	Integer	n		Number of CAI unvalid pixels not processed in GOSAT footprint
gosat_IFOV_Cloud_flags	Integer	n, 16		Number of CAI pixels in GOSAT footprint satisfying each confidence levels (1st level: cloudy, ..., 16th: cloud-free)
gosat_OFOV_Cloud_flags_nyes	Integer	n		Number of CAI valid pixels that match an area that is twice GOSAT footprint (GOSAT 'outer FOV')
gosat_OFOV_Cloud_flags_nno	Integer	n		Number of CAI unvalid pixels not processed in GOSAT outer FOV
gosat_OFOV_Cloud_flags	Integer	n, 16		Number of CAI pixels in GOSAT OFOV satisfying each confidence levels (1st level: cloudy, ..., 16th: cloud-free)
GOSAT_Perc_IFOV_Cloud_free	Float	n		Fraction of IFOV that is cloudfree
GOSAT_Perc_OFOV_Cloud_free	Float	n		Fraction of OFOV that is cloudfree
GOSAT_Cirrus_Flag	Integer	n		0=no cirrus, 1= cirrus
GOSAT_Signal_water_band_2mu	Float	n		Signal in strong water absorbing band around 2 micrometers
ECMWF_Surface_Pressure	Float	n	hPa	Surface pressure
ECMWF_Surface_Temperature	Float	n	K	Surface temperature
GTOPO30_surface_elevation	Float	n	m	Surface elevation
GTOPO30_surface_elevation_min	Float	n	m	Minimum surface elevation in GOSAT footprint

GTOPO30_surface_elevation_max	Float	n	m	Maximum surface elevation in GOSAT footprint
GTOPO30_Surface_Elevation_STDDEV	Float	n	m	Standard deviation in surface elevation within GOSAT footprint
ECMWF_Wind_U	Float	n	m/s	ECMWF surface windseep, zonal direction
ECMWF_Wind_V	Float	n	m/s	ECMWF surface windseep, meridional direction
airmass	Float	n	Molec/ cm^2	Total airmass
airmass_profile	Float	n, nlayers	Molec/ cm^2	Partial column profile
pressure_profile	Float	n, nlayers	hPa	Pressure levels (boundaries of retrieval layers)
nlayers	Integer	1		Number of retrieval layers
nwindow	Integer	1		Number of spectral windows
WVstart_per_Window	Float	nwindow	cm-1	Start wavelength of each window
gosat_SNRpol1_per_Window	Float	n, nwindow		Signal to noise ratio in each window, 1st polarization channel
GOSAT_SNRpol2_per_Window	Float	n, nwindow		Signal to noise ratio in each window, 2nd polarization channel
GOSAT_SIGNALpol1_per_Window	Float	n, nwindow	W/str/cm2/cm-1	Mean signal in each window, 1st polarization channel
GOSAT_SIGNALpol2_per_Window	Float	n, nwindow	W/str/cm2/cm-1	Mean signal in each window, 2nd polarization channel
REMOTEC_Quality_flag	Integer	n		=1 if passed all quality filters, =0 otherwise
REMOTEC_Number_of_Iterations	Integer	n		Number of iterations
REMOTEC_Chi2	Float	n		Total chi^2
REMOTEC_Chi2_per_Window	Float	n, nwindow		Chi^2 in each window
REMOTEC_RMS	Float	n		Root mean square of the fits
REMOTEC_Degree_Of_Freedom_Total	Float	n		Total degree of freedom for signal
REMOTEC_XCO2_Degree_OF_Freedom	Float	n		Degree of freedom for CO2
REMOTEC_XCH4_Degree_OF_Freedom	Float	n		Degree of freedom for CH4
REMOTEC_Aerosols_Degree_OF_Freedom	Float	n		Degree of freedom for aerosols (Full Physics Only)
REMOTEC_SOT_per_Window	Float	n, nwindow		Retrieved optical thickness in each window (Full Physics Only)
REMOTEC_XCO2	Float	n	ppm	Retrieved XCO2
REMOTEC_XCH4	Float	n	ppm	Retrieved XCH4
REMOTEC_XCO2_bias_corrected	Float	n	Ppm	Retrieved XCO2, bias correction applied (Full Physics Only)
REMOTEC_XCH4_bias_corrected	Float	n	ppm	Retrieved XCH4, bias correction applied (Full Physics Only)
REMOTEC_XCO2_uncertainty	Float	n	ppm	Retrieved XCO2 noise error
REMOTEC_XCH4_uncertainty	Float	n	ppm	Retrieved XCH4 noise error
REMOTEC_XCH4_proxy	Float	n	ppm	Proxy XCH4 product (Proxy only)
REMOTEC_XCH4_proxy_uncertainty	Float	n	ppm	Uncertainty (propagation of noise) in the proxy product (Proxy only)
REMOTEC_VMR_CO2_profile	Float	n, nlayers	ppm	Retrieved CO2 mixing ratio Profile
REMOTEC_VMR_CH4_profile	Float	n, nlayers	ppm	Retrieved CH4 mixing ratio profile

REMOTEC_VMR_CO2_profile_uncertainty	Float	n, nlayers	ppm	Retrieved CO2 mixing ratio error profile
REMOTEC_VMR_CH4_profile__uncertainty	Float	n, nlayers	ppm	Retrieved CH4 mixing ratio error profile
REMOTEC_avg_ker_XCO2	Float	n, nlayers		XCO2 column averaging kernels
REMOTEC_avg_ker_XCH4	Float	n, nlayers		XCH4 column averaging kernels
APR_XCO2_CT2010	Float	n	ppm	A priori XCO2 from Carbon Tracker 2010, fields optimized for 2009
APR_XCO2_CORR	Float	N	Ppm	A priori XCO2 from Carbon Tracker 2010 with a correction applied for 2010 and 2011 values (proxy only)
APR_XCH4_TM4	Float	N	Ppm	A priori XCH4 from TM4
APR_VMR_CO2_profile_CT2010	Float	N, nlayers	ppm	A priori CO2 mixing ratio profile
APR_VMR_CH4_profile_TM4	Float	n, nlayers	ppm	A priori CH4 mixing ratio profile
nstate	Integer	1		Number of elements in state vector
REMOTEC_X_STATE_NAME	Float	nstate		Name of all state vector elements
REMOTEC_X_STATE	Float	N,nstate		Retrieved state vector
APR_X_STATE	Float	N,nstate		A priori state vector

Table 8: Additional parameters of the data product generated with the CO2_GOS_SRFP, CH4_GOS_SRFP and CH4_GOS_SRPR algorithms.

14 Appendix G - Additional Constraints Algorithms (ACAs)

14.1 CO2_AIR_NLIS

Mid-to-upper tropospheric integrated content of CO_2 is retrieved from AIRS-AMSU observations using a non-linear regression inverse radiative transfer model using Multi-Layer Perceptrons **/Crevoisier et al., 2004/**. Use is made of 15 AIRS channels located in the 15 µm spectral band that are mostly sensitive to CO_2 and, as all infrared channels, to atmospheric temperature. Observations made in the microwave by the AMSU instrument, flying with AIRS onboard MetOp-A (both instruments are synchronized), are also sensitive to temperature, but are insensitive to CO_2. Thus, combining AIRS and AMSU allows separating the two signals. Potential radiative systematic biases existing between simulations used to train the networks and observations are computed for each channel by averaging, over three years of operation, the differences between simulations and collocated (in time and space) satellite observations. The simulations are performed using the 4AOP forward model **/Scott and Chédin, 1981/**; http://www.noveltis.net/4AOP/, which is based on the GEISA spectroscopic database (available at http://ether.ipsl.jussieu.fr/) **/Jacquinet-Husson et al., 2010/**, and radiosonde measurements from the Analyzed RadioSoundings Archive database (available at http://ara.lmd.polytechnique.fr) as inputs.

The current data format is ASCII, but can be modified according to user need. One file corresponds to one month. The data files contain header lines providing information on the version, the month and the pressure levels used in the retrieval. They are followed by the retrieval which are provided for each cloud-free AIRS FOV, with the following format: yymmdd, land/sea index, angle of observation, hhmmss, latitude, longitude, integrated content, associated error, weighting function.

14.2 CO2_IAS_NLIS

Mid-to-upper tropospheric integrated content of CO_2 is retrieved from IASI-AMSU observations using a non-linear regression inverse radiative transfer model using Multi-Layer Perceptrons **/Crevoisier et al., 2009a/**. Use is made of 9 IASI channels located in the 15 µm spectral band that are mostly sensitive to CO_2 and, as all infrared channels, to atmospheric temperature. Observations made in the microwave by the AMSU instrument, flying with IASI onboard MetOp-A (both instruments are synchronized), are also sensitive to temperature, but are insensitive to CO_2. Thus, combining IASI and AMSU allows separating the two signals. Potential radiative systematic biases existing between simulations used to train the networks and observations are computed for each channel by averaging, over the first three years of operation (July 2007–August 2010), the differences between simulations and collocated (in time and space) satellite observations. The simulations are performed using the 4AOP forward model **/Scott and Chédin, 1981/**; http://www.noveltis.net/4AOP/, which is based on the updated 2009 version of the GEISA spectroscopic database (available at http://ether.ipsl.jussieu.fr/) **/Jacquinet-Husson et al., 2010/**, and radiosonde measurements from the Analyzed RadioSoundings Archive database (available at http://ara.lmd.polytechnique.fr) as inputs.

The current data format is ASCII, but can be modified according to user need. One file corresponds to one month. The data files contain header lines providing information on the version, the month and the pressure levels used in the retrieval. They are followed by the retrieval which are provided for each cloud-free IASI FOV, with the following format: yymmdd, land/sea index, angle of observation, hhmmss, latitude, longitude, integrated content, associated error, weighting function.

14.3 CH4_IAS_NLIS

Mid-tropospheric integrated content of CH_4 is retrieved from IASI-AMSU observations using a non-linear regression inverse radiative transfer model using Multi-Layer Perceptrons **/Crevoisier et al., 2009b/**. Use is made of 10 IASI channels located in the 7.7 µm spectral band that are mostly sensitive to CH_4 and, as all infrared channels, to atmospheric temperature. Observations made in the microwave by the AMSU instrument, flying with IASI onboard MetOp-A (both instruments are synchronized), are also sensitive to temperature, but are insensitive to CH_4. Thus, combining IASI and AMSU allows separating the two signals. Potential radiative systematic biases existing between simulations used to train the networks and observations are computed for each channel by averaging, over the first three years of operation (July 2007–August 2010), the differences between simulations and collocated (in time and space) satellite observations. The simulations are performed using the 4AOP forward model **/Scott and Chédin, 1981/**; http://www.noveltis.net/4AOP/, which is based on the updated 2009 version of the GEISA spectroscopic database (available at http://ether.ipsl.jussieu.fr/) **/Jacquinet-Husson et al., 2010/**, and radiosonde measurements from the Analyzed RadioSoundings Archive database (available at http://ara.lmd.polytechnique.fr) as inputs.

The current data format is ASCII, but can be modified according to user need. One file corresponds to one month. The data files contain header lines providing information on the version, the month and the pressure levels used in the retrieval. They are followed by the retrieval which are provided for each cloud-free IASI FOV, with the following format: yymmdd, land/sea index, angle of observation, hhmmss, latitude, longitude, integrated content, associated error, weighting function.

14.4 CO2_ACE_CLSR

As described in **/Foucher et al. 2009, 2010/**, the methodology used to determine CO_2 profiles (5-25 km) from ACE-FTS observations has two main steps: (i) pointing parameter estimation (tangent heights, pressure and temperature profiles); (ii) CO_2 vertical profile estimation using a careful selection of CO_2 spectral micro-windows. Both steps use a similar constrained least-squares retrieval method. The target variable is a vector containing tangent heights and a temperature profile in the first step or a CO_2 concentration vertical profile in the second step. The accurate determination of the instrument pointing parameters (tangent heights) and pressure/ temperature profiles is performed independently from an a priori CO_2 profile, using, for the first time, the N_2 collision induced continuum absorption near 4 µm, with a high precision (50 m standard deviation). The vertical resolution of the retrieved CO_2 profile is around 2 km for the lowest altitudes and about 2.5 km at 15 km. The estimated

CO_2 total error is characterized by a bias of about 1 ppm and a standard deviation of about 2 ppm after averaging over 20 spatially and temporally consistent profiles.

14.5 CH4_MIP_IMK

MIPAS CH_4 retrievals produced at IMK are based on constrained least squares fitting of simulated spectra to measured spectral radiances in the 1220-1305 cm^{-1} spectral region. The reported geophysical quantity is volume mixing ratio versus altitude. The temperature (retrieved from MIPAS spectra) and the pressure (hydrostatical, based on MIPAS temperatures) are provided along with the CH_4 data in order to allow transformation to different representations (e.g. number density versus pressure or versus potential temperature). The data are retrieved on a fixed altitude grid of 1 km spacing below 44 km and 2 km above 44 km, i.e. the grid is independent of the actual tangent altitudes of the measurement. Along with the data, the diagonal values of the averaging kernels matrix are provided, as well as the measurement noise (in terms of the diagonal entries of the covariance matrix). Full measurement error covariance matrices and averaging kernel matrices are stored and can be made available on request, as well as parameter error estimates.

Besides the averaging kernel diagonal, the estimate of the altitude resolution and the retrieval errors, the following quality indicator are reported: the lowermost tangent altitude of the limb scan used; spectra contaminated by cloud signal are discarded from analysis, and thus there is zero measurement information in the profile below this altitude. A priori profiles are not reported because the constraint applied for CH_4 is Tikhonov type first order difference smoothing with zero slope, hence the a priori is constant zero.

The exported data are stored in daily ASCII files, structured by $-signs at the very first position of a line. Each $-sign marks a new item/entry in the file. Numbers immediately following the $-sign give paragraph, section, subsection, and clause of the corresponding entry.

The files contain profiles together with visibility flags, corresponding geolocations, date/time, latitude/longitude of the projection of the scan on the Earth surface, solar zenith angle, engineering tangent altitude, grid altitude, pressure and temperature, as well as diagnostics of the retrieval success: degree of freedom, chi2, rms, diagonal of averaging kernel matrix, vertical resolution from AKM columns, and the noise error.

14.6 CH4_SCI_ONPD

The SCIAMACHY Solar Occultation CH_4 product (CH4_SCI_ONPD) is derived by an onion peeling DOAS method. The native results are vertical number density profiles on a 1 km grid with a vertical resolution of about 4 km. The number densities are converted to VMRs using collocated ECMWF pressure and temperature data. The product is still under development and not yet released to the public; therefore the format might change in the future.

The current data format is (gzipped) ASCII. There is one file per measurement/profile. The file naming convention is as follows:

SCIA_occ_yyyymmdd_HHMMSS_1_0_OOOOO.ch4.vmr.gz

where yyyy=year, mm=month, dd=day, HH=hour, MM=minute, SS=second, OOOOO=orbit number denote the start time and orbit number of the measurement.

The data files contain comment/header lines which are marked with a leading '#'.The header entries are described in Table 8. There is one data line for each tangent altitude. The columns of the data lines are:

- layer no.
- tangent altitude (km)
- retrieved number density (mol/cm^3)
- error on retrieved number density (mol/cm^3)
- derived CH_4 VMR (ppmv)
- water vapour number density (mol/cm^3) from matching ECMWF data (not relevant for CH_4)
- ECMWF pressure (hPa)
- ECMWF temperature (K)

Important notes:

- Although the data files contain values for altitudes between 0 and 50 km, only data between 20 and 40 km should be used. The other data are not reliable, especially below 15 km no retrieval is performed at all.

- The number density error is only a rough estimate based on the individual fit residuals. It does not consider effects of e.g. vertical smoothing and saturation correction (applied after the fit). The 'real' errors are probably smaller.

Mark	Example	Description
# state_start	02-Aug-2002 01:15:31.197545	Start date and time of measurement
# center_lat_lon (deg)	51.700 277.265	Geolocation of center point
# corner_lat_lon (deg)	51.462 277.260 51.489 277.198 52.284 277.143 52.308 277.087	Corner coordinates of ground pixel
# Program Version	3.2	Retrieval program version number
# Product Version	3.2.1	Data product version number
# filename	SCIA_occ_20020802_011531_1_0_02204.occ	Input filename
# no. of absorbers	3	Number of absorbers considered in the fit
# alphafile[0]	/tmp/noel/RTM/Alpha_rad.ch4	RTM data base of first absorber (CH4)
# alphafile[1]	/tmp/noel/RTM/Alpha_rad.co2	RTM data base of second absorber (CO2)
# alphafile[2]	/tmp/noel/RTM/Alpha_rad.T	RTM data base of third absorber (T)
# top minlam (nm)	1559.00	Minimum wavelength of fit window at highest altitude
# top maxlam (nm)	1671.00	Maximum wavelength of fit window at highest altitude
# low minlam (nm)	1559.00	Minimum wavelength of fit window at lowest altitude
# low maxlam (nm)	1671.00	Maximum wavelength of fit window at lowest altitude
# min. tangent height (km)	15.00	Tangent height below which no retrieval is performed
# no. of orig. meas. alt.	20	Number of altitudes of original measurements
# orig. meas. altitudes (km)	4.93 7.29 9.66 12.02 14.37 16.85 19.52 23.09 25.74 28.40 31.11 34.65 37.41 40.04 42.73 46.25 48.93 51.60 54.27 57.76	Altitudes of original measurements (km)
# ECMWF file	/home/Data/Occ/Operational_CO2_CH4/Scripts/../ECMWF/./Profiles/2002/08/02/ecmwf_h2o_profile.2002080200.Lat_026.Lon_185	ECMWF file name used for p, T
# tropopause_height (km)	11.25	Estimated tropopause height from ECMWF data
# tropopause_temp (K)	221.40	Estimated tropopause temperature from ECMWF data
# No., h_scia(km), n_scia(mol/cm3), nerror_scia(mol/cm3), VMR_scia[ppmv],		Comment line, explaining the format of the data lines

n_ecmwf(mol/cm3), p_ecmwf[hPa], T_ecmwf[K]		
# smoothing width (km)	4.100000	Width of boxcar smoothing applied to the data after the retrieval
# satcorr file 0	/home/Data/Occ/Operational_CO2_CH4/Scripts/../Corr/satcorr.ch4	File used for saturation correction of first absorber (CH4)
# satcorr file 1	/home/Data/Occ/Operational_CO2_CH4/Scripts/../Corr/satcorr.co2	File used for saturation correction of second absorber (CO2)
# co2corr file 0	/home/Data/Occ/Operational_CO2_CH4/Scripts/../Corr/co2corr.dat	File used for CO2 correction of first absorber (CH4)

Table 9: Header of CH4_SCI_ONPD files.

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