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	Proposed final draft of Version 1	Includes inputs received from project team and feedback from Draft 2

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1 Overview

This document is Product Specification Document Version 1 (PSDv1), 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, 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 EVC 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 23 January 2009 **/Yokota2009/** by JAXA, the Japanese Space Agency. GOSAT provides the first dedicated global measurements of total column CO2and CH4 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 0.3cm^{-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 CO2 at a 100-1000~km spatial resolution **/Kuze2009/**. The aim for CH4 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 sunglint mode over the ocean within ±20° of the subsolar 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.

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

4 ECV Core Algorithms (ECAs)

ECV Core Algorithms (ECAs) are algorithms to retrieve XCO_2 and/or XCH_4 from SCIAMACHY and/or TANSO. 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) 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., 2010	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., 2010	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_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, used a-priori profiles, etc.

In order to provide this and allow comparison during the Round-Robin phase, all ECAs are expected to contain the parameters found in the table below.

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	A priori XCO2 (ppm) or

			ppb (CH4)	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.

As BESD is still under development, its data product format is not yet finally defined. However, in the following, a description is given defining the planned data format.

8.1 Data organization

The data organization will follow the common definitions given in this document for all ECV core algorithms. All retrievals of a single orbit which pass initial quality checks will be packed into an individual NetCDF file.

8.1.1 File naming convention

As commonly defined within this document (see Section 3).

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 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 WFMDv2.0 described in **/Schneising et. al, 2010/**.

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

The data organization will follow the common definitions given in this document for all ECV core algorithms.

9.1.1 File naming convention

As commonly defined within this document (see Section 3).

9.1.2 Common data fields

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

9.1.3 Algorithm specific data fields

There will be additional data fields based on the current version WFMDv2.0 as specified in Table 4. This list of data fields may be subject to changes during the project.

10 Appendix C - CH4_SCI_WFMD

The current version is WFMDv2.0 described in **/Schneising et. al, 2010/**.

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

The data organization will follow the common definitions given in this document for all ECV core algorithms.

10.1.1 File naming convention

As commonly defined within this document (see Section 3).

10.1.2 Common data fields

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

10.1.3 Algorithm specific data fields

There will be additional data fields based on the current version WFMDv2.0 as specified in table. This list of data fields may be subject to changes during the project.

Name	Type	Dimen sions	Units	Description
px#	tbs	tbs	tbs	Ground pixel number (per orbit)
st#	tbs	tbs	tbs	State number [-] (0,1,..)
read#	tbs	tbs	tbs	Ground pixel number (per state) [-] (0,1,...)
t	tbs	tbs	tbs	Pixel type [-] (1:forward 2:backscan)
t_int	tbs	tbs	tbs	Integration time [s]
cld	tbs	tbs	tbs	PMD cloud mask (1:probably cloud contaminated)
lnd	tbs	tbs	tbs	Land mask (1:completely land covered)
snrad	tbs	tbs	tbs	Sun-normalized radiance (R/I*PI) [-]
alt	tbs	tbs	tbs	Average ground altitude [km]
H2O(CH4 fit)	tbs	tbs	tbs	H2O column of CH4 fit [molec./cm2]
H2O_err(CH4)	tbs	tbs	tbs	H2O column error of CH4 fit [%]
H2O(CO2 fit)	tbs	tbs	tbs	H2O column of CO2 fit [molec./cm2]
H2O_err(CO2)	tbs	tbs	tbs	H2O column error of CO2 fit [%]
O2#	tbs	tbs	tbs	Number of O2 (sub-)pixel [-]
O2	tbs	tbs	tbs	O2 column [molec./cm2]
O2_err	tbs	tbs	tbs	O2 column error [%]
O2_rms	tbs	tbs	tbs	RMS of O2 fit residuum [-]
O2Q	tbs	tbs	tbs	O2 quality flag (0:good 1:bad)
CO2#	tbs	tbs	tbs	Number of CO2 (sub-)pixel [-]
CO2	tbs	tbs	tbs	CO2 column [molec./cm2]
CO2_err	tbs	tbs	tbs	CO2 column error [%]
CO2_rms	tbs	tbs	tbs	RMS of CO2 fit residuum [-]
CO2Q	tbs	tbs	tbs	CO2 quality flag (0:good 1:bad)
XCO2Q	tbs	tbs	tbs	XCO2 quality flag (0:good 1:bad)
CH4_rms	tbs	tbs	tbs	RMS of CH4 fit residuum [-]
CH4Q	tbs	tbs	tbs	CH4 quality flag (0:good 1:bad)
XCH4Q	tbs	tbs	tbs	XCH4 quality flag (0:good 1:bad)
XCO2FQ	tbs	tbs	tbs	XCO2 final quality flag (0:good 1:bad)
XCH4FQ	tbs	tbs	tbs	XCH4 final quality flag (0:good 1:bad)
XCH4_corr	tbs	tbs	tbs	XCH4 CarbonTracker-corrected [ppb]

Table 4: Additional parameters of the data product generated with the CO2_SCI_WFMD and CH4_SCI_WFMD algorithm. tbs = to be specified.

11 Appendix D - CO2_GOS_OCFP and CH4_GOS_OCFP

This section provides the full product description for the CO2_GOS_OCFP and CH4_GOS_OCFP 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) was developed 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, allowing a full year of data to be retrieved.

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 orbit which converge and pass initial quality checks are packaged into a single NetCDF file.

11.2 File naming convention

The GOSAT L1B naming convention is as follows:
GOSATTFTS_yyyymmddhhMMPPPSSSX_1BTTTTVVVVVV
Table X 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

The CO2_GOS_OCFP and CH4_GOS_OCFP 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_yyyymmddhhMMPPP_<processor_version>_<unique_tracking_id>
CH4_GOS_OCFP_yyyymmddhhMMPPP_<processor_version>_<unique_tracking_id>

The guidelines from the Collocation Meeting recommend that “CCI data should include a unique tracking ID for each data product file in the file metadata”. We also intend to use this number in the filename itself.

11.3 Data Contents

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

Name	Type	Dimensions	Units	Description
n	Integer	1		Number of exposures in file
m	Integer	1		Number of retrieval levels
instrument	String	1		“GOSAT”
l2_processing_institute	String	1		“ULE”
l2_processor_version	String	1		Version Number of University of Leicester L2 Retrieval
Exposure_ID	String	n		Unique identification for exposure, see Section XX for naming convention
L1B_Observation_Type	String	n		Observsation type of L1B data. Options:

				'OB1D', 'OB1N', 'OB2D', 'SPOD', 'SPON', 'CALM', 'LUCA'
L1B_Version_Number	String	n		Version number for L1B data
Cross-Track_Points	Integer	n		Number of cross-track measurement points. Options: 1,3,5,7,9
latitude_centre	Float	n	Degrees	Latitude of pixel centre
longitude_centre	Float	n	Degrees	Longitude of pixel centre
longitude_corners	Float	n x 4	Degrees	Longitude of pixelextremes
latitude_corners	Float	n x 4	Degrees	Latitude of pixel extremes
time	Double	n	Seconds	seconds since 01.01.1970 00:00 UTC
Year	String	n	(UTC)	Year of measurement (yyyy)
Month	String	n	(UTC)	Month of measurement (mm)
Day	String	n	(UTC)	Day of measurement (dd)
Hour	String	n	(UTC)	Hour of measurement (hh)
Min	String	n	(UTC)	Minute of measurement (MM)
Sec	String	n	(UTC)	Second of measurement (ss)
solar_zenith_angle	Float	n	degrees	Solar Zenith Angle (0°=zenith)
viewing_zenith_angle	Float	n	degrees	Viewing Zenith Angle(0°=zenith)
azimuth_difference	Float	n	degrees	Azimuth Difference (0°=zenith)
at_angle	Float	n	degrees	Measurement along-track angle
ct_angle	Float	n	degrees	Measurement cross-track angle
at_angle_error	Float	n	degrees	Error in along-track angle
ct_angle_error	Float	n	degrees	Error in cross-track angle
atn_lat	Float	n	degrees	Along Track (Negative Direction) Latitude Point
atn_lon	Float	n	degrees	Along Track (Negative Direction) Longitude Point
atp_lat	Float	n	degrees	Along Track (Positive Direction) Latitude Point
atp_lon	Float	n	degrees	Along Track (Positive Direction) Longitude Point
ctn_lat	Float	n	degrees	Cross Track (Negative Direction) Latitude Point
ctn_lon	Float	n	degrees	Cross Track (Negative Direction) Longitude Point
ctp_lat	Float	n	degrees	Cross Track (Positive Direction) Latitude Point
ctp_lon	Float	n	degrees	Cross Track (Positive Direction) Longitude Point
Xtarget	Float	n	ppm	Retrieved XCO2 (ppm) or XCH4 (ppb)
Xtarget_uncertainty	Float	n	ppm	Uncertainty in retrieved XCO2 (ppm) or XCH4 (ppb)
xtarget_smoothing_error	Float	n	ppm	Retrieved XCO2 or XCH4 Smoothing Error
xtarget_noise_error	Float	n	ppm	Retrieved XCO2 or XCH4 Noise Error
xtarget_interference_error	Float	n	ppm	Retrieved XCO2 or XCH4 Interference Error
Retrieved_Psurf	Float	n	hPa	Retrieved Surface pressure

normalised_ column_averaging_kernel	Float	n x m		Normalised Column Averaging Kernel Profile
retr_aero1	Float	n		Retrieved Total Aerosol1 AOD
retr_aero2	Float	n		Retrieved Total Aerosol2 AOD
retr_aero2	Float	n		Retrieved Total IC AOD
snr1	Float	n		Signal-to-Noise Ratio of Band 1
snr2	Float	n		Signal-to-Noise Ratio of Band 2
snr3	Float	n		Signal-to-Noise Ratio of Band 3
total_chisq	Float	n		Chi-Square of fit residual
total_rms	Float	n		RMS of fit residual
rms1	Float	n		RMS of Band 1
rms2	Float	n		RMS of Band 2
rms3	Float	n		RMS of Band 3
chisq1	Float	n		CHISQ of Band 1
chisq2	Float	n		CHISQ of Band 2
chisq3	Float	n		CHISQ of Band 3
num_iterations	Integer	n		Number of iterations performed
num_divs	Integer	n		Number of divergences
outcome	Integer	n		1: pass 2: fail 3: max iterations exceed 4: max divergences exceed
conv_flag	Integer	n		0: Not Converged 1: Converged
cost_div	Integer	n		0: No Divergence 1: Divergence
Pressure_levels	Float	n x m	hPa	Retrieval pressure levels
ap_temp_profile	Float	n x m	K	Apriori Temperature Profile
ap_h2o_profile	Float	n x m	ppm	Apriori H2O Profile
ap_co2_profile	Float	n x m	ppm	Apriori CO2 Profile
surface_elevation	Float	n	km	Mean surface elevation of pixel
surface_elevation_std	Float	n	km	Standrd Deviation of mean surface elevation of pixel
psurf	Float	n	hPa	Surface Pressure
psur_std	Float	n	hPa	Standard Deviation of Surface Pressure over pixel
retr_co2_profile	Float	n x m	ppm	Retrieved CO2 Profile
retr_co2_profile_error	Float	n x m	ppm	Retrieved CO2 Profile Error
retr_disp	Float	n		Retrieved Dispersion
retr_disp_error	Float	n		Retrieved Dispersion Error
retr_albedo	Float	n		Retrieved Albedo
retr_albedo_error	Float	n		Retrieved Albedo Error
retr_ic_profile	Float	n x m		Retrieved ice-cloud Profile
retr_ic_profile_error	Float	n x m		Retrieved ice_cloud Profile Error
retr_aero1_profile	Float	n x m		Retrieved Aerosol1 Profile
retr_aero1_profile_error	Float	n x m		Retrieved Aerosol1 Profile Error
retr_aero2_profile	Float	n x m		Retrieved Aerosol2 Profile
retr_aero2_profile_error	Float	n x m		Retrieved Aerosol2 Profile

				Error
retr_temp	Float	n		Retrieved Temperature Scale Factor
retr_temp_error	Float	n		Retrieved Temperature Scale Factor Error
retr_h2o	Float	n		Retrieved H2O Scale Factor
retr_h2o_error	Float	n		Retrieved H2O Scale Factor Error
retr_ch4	Float	n		Retrieved CH4 Scale Factor
retr_ch4_error	Float	n		Retrieved CH4 Scale Factor Error
retr_psurf_error	Float	n		Retrieved Psurf Error

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 HDF5 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_SRON_CH4_vXX_1PUDPA20100101_002615_000060322085_00346_40981_1171.h5
with vXX denoting the version number.

12.3 Data Contents

The following table details the content of each HDF5 file (containing n retrievals).

Name	Type	Dimensions	Units	Description
/Data/Geolocation				
Latitude	Float	n	degrees	Geodetic latitude of pixel centre
Longitude	Float	n	degrees	Geodetic longitude of pixel centre
LineOfSightZenithAngle	Float	n	degrees	Line of sight zenith angle
SolarZenithAngle	Float	n	degress	Solar zenith angle
IntegrationTime	Float	n	seconds	Integration time
CornerLatitudes	Float	(n,4)	degrees	Latitude of the 4 corners of the ground-pixel
CornerLongitudes	Float	(n,4)	degrees	Longitude of the 4 corners of the ground-pixel
SurfaceElevation	Float	n	meter	Ground pixel surface elevation
AirMassFactor	Float	n	Modified julian day	Sounding time
OrbitalPhase	Float	n		orbital phase (from L1B file)
ScanRange	Float	n	Degree	Absolute range of line of sight zenith angles
state_id	Float	n		Measurement state id (from L1B file)
/Data/FitResults				
VCD_CH4	Float	n	molec/cm^2	Methane vertical column density
VCD_CH4_ERROR	Float	n	molec/cm^2	1-sigma precision error in methane vertical column density
VCD_CO2	Float	n	molec/cm^2	Carbon dioxide vertical column density
VCD_CO2_ERROR	Float	n	molec/cm^2	1-sigma precision error in CO_2 vertical column density
xVMR_CH4	Float	n	ppb	Derived column averaged dry methane mixing ratio
xVMR_CH4_1sigma	Float	n	ppb	1-sigma precision error in xVMR_CH4
VCD_CO2_MODEL	Float	n	molec/cm^2	model CO2 vertical column density used to derive xCH_4
/Data/ECMWF				
DryColumn	Float	n	molec/cm^2	Total vertical column density of all gases except water (from ECMWF)
WaterColumn	Float	n	molec/cm^2	vertical column density of water (from ECMWF)
SurfacePressure	Float	n	hPa	surface pressure (from ECMWF)
SurfaceTemperature	Float	n	K	Surface temperature (from ECMWF)
/Data/AveragingKernel				

CarbonDioxideAK	Float	n x m	-	CO_2 total column averaging kernel for 12 layers per sounding
MethaneAK	Float	n x m	-	CH_4 total column averaging kernel for 12 layers per sounding
CarbonDioxidePrior	Float	n x m	-	CO_2 prior profile (12 layers)
MethanePrior	Float	n x m	-	CH_4 prior profile (12 layers)
Pressure	Float	n x m	hPa	corresponding pressure profile for the averaging kernels (12 layers per sounding)
/Data/Auxiliary				
residual_ch4_1	Float	n	-	fit residual RMS for the CH_4 fit window
residual_ch4_2	Float	n	-	fit reduced chi^2 for the CH_4 fit window
residual_co2_1	Float	n	-	fit residual RMS for the CO_2 fit window
residual_co2_2	Float	n	-	fit reduced chi^2 for the CO_2 fit window
iterations_ch4	Float	n	ppm	number of iterations used in the CH_4 fit
iterations_co2	Float	n	hPa	number of iterations used in the CO_2 fit
BU_ch4_window	Float	n		raw detector readout at first pixel in CH_4 window
BU_co2_window	Float	n		raw detector readout at first pixel in CO_2 window
pixels_ch4	Float	n	-	number of spectral pixels in CH_4 fit window
pixels_co2	Float	n	-	number of spectral pixels in CO_2 fit window

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 passed 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 a single day will be saved in a single NetCDF file.

The following table 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 O_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).
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, retrieved optical thickness, and aerosols parameters are irrelevant and not provided. We additionally provide the quantity XCH4_proxy=XCH4/XCO2 *XCO2_apr.

Name	Type	Dim.	Units	Description
n	Integer	1		Number of exposures in file
l1b_input_filename	String	n		GOSAT L1B filenames, format GOSATTFTS_yyyymmddhhMMPPPSSSX_1BTTTTVVVVVV.01 (see table in section Appendix A)
gosat_idexpo	Integer	n		Exposure index number
gosat_obsmode	String	n		Observation mode: 'OB1D', 'OB1N', 'OB2D', 'SPOD', 'SPON', 'CALM', 'LUCA'
gosat_gain	String	n		Observation gain: 'HH','MM'
gosat_sunglint	Integer	n		0 = Nadir, 1 = Glint
Longitude_centre	Float	n	degrees	Centre Longitude
Latitude_corners	Float	4*n	degrees	Latitude extremes in GOSAT FOV
Instrument_Azimuth_Angle	Float	n	degrees	Satellite azimuth angle

gosat_cld_ifov_nyes	Integer	n		Number of CAI pixels that match GOSAT footprint
gosat_cld_ifov_nno	Integer	n		Number of CAI pixels not processed in GOSAT footprint
gosat_cld_ifov_flag	Integer	n, 16		Number of CAI pixels in GOSAT footprint satisfying each confidence levels (1st level: cloudy, ..., 16th: cloud-free)
gosat_cld_ofov_nyes	Integer	n		Number of CAI pixels that match an area that is twice GOSAT footprint (GOSAT 'outer FOV')
gosat_cld_ofov_nno	Integer	n		Number of CAI pixels not processed in GOSAT outer FOV
gosat_cld_ofov_flag	Integer	n, 16		Number of CAI pixels in GOSAT OFOV satisfying each confidence levels (1st level: cloudy, ..., 16th: cloud-free)
meteo_psfmet	Float	n	hPa	Surface pressure
meteo_tsfmet	Float	n	K	Surface temperature
meteo_surface_elevation	Float	n	m	Surface elevation
meteo_min_surface_elevation	Float	n	m	Minimum surface elevation in GOSAT footprint
meteo_max_surface_elevation	Float	n	m	Maximum surface elevation in GOSAT footprint
meteo_airmass	Float	n	Molec/cm^2	Total airmass
meteo_air_profile	Float	n, m	Molec/cm^2	Partial column profile
meteo_pressure_levels	Float	n, m	hPa	Pressure levels (boundaries of retrieval layers)
ini_nlay	Integer	n		Number of retrieval layers
ini_nwin	Integer	n		Number of spectral windows
ini_wstart_win	Float	n, ini_nwin	cm-1	Start wavelength of each window
gosat_pol01snr_win	Float	n, ini_nwin		Signal to noise ratio in each window, 1st polarization channel
Chi2	Float	n		Total chi^2
DFS_aero	Float	n		Degree of freedom for aerosols
inv_sot_win	Float	n, ini_nwin		Retrieved optical thickness in each window
inv_XCO2	Float	n	ppm	Retrieved XCO2
inv_XCH4	Float	n	ppm	Retrieved XCH4
inv_XCO2_uncertainty	Float	n	ppm	Retrieved XCO2 noise error
inv_XCH4_uncertainty	Float	n	ppm	Retrieved XCH4 noise error
inv_H2O_column	Float	n	Molec/cm^2	Retrieved H2O total column
inv_VMR_profile_CO2	Float	n, m	ppm	Retrieved CO2 mixing ratio Profile
inv_VMR_profile_CH4	Float	n, m	ppm	Retrieved CH4 mixing ratio profile
inv_VMR_profile_CO2_uncertainty	Float	n, m	ppm	Retrieved CO2 mixing ratio error profile
inv_VMR_profile_CH4__uncertainty	Float	n, m	ppm	Retrieved CH4 mixing ratio error profile
inv_avg_ker_CO2_profile	Float	n, m* m		Averaging kernels for CO2 mixing ratio profile
inv_avg_ker_CH4_profile	Float	n, m* m		Averaging kernels for CH4 mixing ratio profile
inv_avg_ker_XCO2	Float	n, m		XCO2 column averaging kernels
inv_avg_ker_XCH4	Float	n, m		XCH4 column averaging kernels
inv_alb_win_order00	Float	n, ini_nwin		Retrieved 0th order albedo per

				window
inv_alb_win_order01	Float	n, ini_nwin		Retrieved 1st order albedo per window
inv_ioff_win_order00	Float	n		Retrieved intensity offset in window 1
inv_shift_win_order00	Float	n, ini_nwin	cm-1	Retrieved spectral shift of FTS spectra per window
inv_xsshift_win_order00	Float	n, ini_nwin	cm-1	Retrieved spectral shift of cross-sections per window
inv_aero_amount	Float	n	particles/cm^2	Retrieved total column number density for aerosols
inv_aero_height	Float	n	m	Retrieved height distribution parameter for aerosols
inv_aero_size	Float	n		Retrieved size distribution parameter for aerosols
XCO2_apriori	Float	n	ppm	A priori XCO2
VMR_profile_CH4_apriori	Float	n, m	ppm	A priori CH4 mixing ratio profile
apr_H2O_column	Float	n	Molec/ cm^2	A priori H2O total column
apr_alb_win_order00	Float	n, ini_nwin		A priori 0th order albedo per window
apr_alb_win_order01	Float	n, ini_nwin		A priori 1st order albedo per window
apr_ioff_win_order00	Float	n		A priori intensity offset in window 1
apr_shift_win_order00	Float	n, ini_nwin	cm-1	A priori spectral shift of FTS spectra per window
apr_xsshift_win_order00	Float	n, ini_nwin	cm-1	A priori spectral shift of cross-sections per window
apr_aero_amount	Float	n	particles/cm^2	A priori amount parameter for aerosols
apr_aero_height	Float	n	m	A priori height distribution parameter for aerosols
apr_aero_size	Float	n		A priori size distribution parameter for aerosols

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 AIRS-AMSU observations using a non-linear regression inverse radiative transfer model using Multi-Layer Perceptrons **/Crevoisier et al., 2009a/**. Use is made of 9 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 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 CH4 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 5. 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),		Comment line, explaining the format of the

nerror_scia(mol/cm3), VMR_scia[ppmv], n_ecmwf(mol/cm3), p_ecmwf[hPa], T_ecmwf[K]		data lines
# 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 5: Header of CH4_SCI_ONPD files.

End of document