ESA Climate Change Initiative (CCI)

Product Specification Document (PSD)

for the Essential Climate Variable (ECV)

Greenhouse Gases (GHG)

- Description of Common Parameters for core (ECA) products -

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1 Overview

This document is Product Specification Document (PSD) Version 3 (PSDv3), which is a deliverable of the ESA project GHG-CCI (http://www.esa-ghg-cci.org).

This version of the PSD incorporates the user requirements as described in the GHG-CCI User Requirements Document (URD) **/Buchwitz et al., 2011/** as well as the Data Standards Requirements for CCI Data Producers **/Bennett and James, 2013/**.

The GHG-CCI project aims at generating and delivering the Essential Climate Variable (ECV) Greenhouse Gases (GHG) in-line with GCOS (Global Climate Observing System) requirements **/GCOS 2011/**. GHG-CCI addresses the ECV "Greenhouse Gases" defined as by GCOS follows: "Retrievals of greenhouse gases, such as CO_2 and CH_4, of sufficient quality to estimate regional sources and sinks".

Two kinds of algorithms are used within GHG-CCI to generate satellite-derived atmospheric carbon dioxide (CO_2) and methane (CH_4) data products:

- **ECV Core Algorithms (ECAs):** Algorithms to retrieve column-averaged dry air mole fractions of CO_2 and CH_4 from (currently) 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. Please see **Table 1** for an overview about all products generated with ECAs.
- 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 and MIPAS. This can provide additional constraints for inverse modelling of CO_2 and/or CH_4 regional fluxes by providing atmospheric CO_2 and/or CH_4 information for "upper layers".

In this document only the GHG-CCI ECA products are described. Furthermore, this PSD only describes the "common parameters" of all ECA products, i.e., those parameters, which are common to all ECA products. The individual ECA products typically have additional, algorithm specific parameters. **These specific parameters are not described in this document but are / will be described in dedicated Product User Guides (PUGs)** (see GHG-CCI website).

ACA product formats will not be described in this document but in dedicated PUGs (see GHG-CCI website).

Currently GHG-CCI is in Phase 2 (2014-2016). Previous versions of this document (PSDv1 and PSDv2) describe the products generated during Phase 1 of GHG-CCI (2010-2013). In particular PSDv2 describes the format of the first version of the GHG-CCI Climate Research Data Package (CRDP#1).

This document (**PSDv3**) describes the improved format for GHG-CCI core (=ECA) products to be used for the next version of the CRDP, which is **CRDP#2** (planned to be available in October 2014).

These products plus corresponding documentation will be available for download via the same website as used for all GHG-CCI products (including previous versions, i.e., CRDP#1):

http://www.esa-ghg-cci.org/ -> CRDP (Data)

An overview of all GHG-CCI data products (ECA and ACA products) including data access info etc. is given on the **GHG-CCI main data products website**:
http://www.esa-ghg-cci.org/ -> CRDP (Data) -> GHG-CCI Data Products Main Website

For a short overview of all ECA products please see **Table 1**. As can be seen, **Table 1** lists baseline and alternative algorithms.

The purpose of the alternative products is to "challenge the baseline" but also to provide alternative products for ensemble applications. If it will be shown in the future that the alternative algorithm/product is better than the baseline, the baseline will change.

Focus of GHG-CCI Phase 2 (2014-2016) will be on the **baseline products** (full documentation, product format meeting all requirements, data available in time as planned, entire planned time series processed, etc.); the **alternative and EMMA products** will also be further developed but with lower priority. For the actual status please visit the GHG-CCI main data products website (see above).

The main purpose of this document is to describe the new data format for ECA products (limited to common parameters) to be used for the CRDP#2 (planned release October 2014). All baseline products will be in this new format but not necessarily all alternative products and the EMMA product (although GHG-CCI will aim at achieving this).

Product format changes in the future (if any) will be reflected in future updates to this document.

ECA products: GHG-CCI Core Products						
Product Main ID	**Product**	**Product details**	**Sensor**	**Algorithm**		**Comment**
				Baseline	**Alternative (*)**	
XCO2_SCI	XCO_2	Level 2, CO_2 column-averaged dry-air mole fraction (in ppm)	SCIAMACHY / ENVISAT	BESD	WFMD	
XCO2_GOS	XCO_2	Level 2, CO_2 column-averaged dry-air mole fraction (in ppm)	TANSO / GOSAT	OCFP (UoL-FP), SRFP (RemoTeC) (baseline not yet defined (#))		
XCO2_EMMA	XCO_2	Level 2, CO_2 column-averaged dry-air mole fraction (in ppm)	SCIAMACHY and GOSAT	EMMA (*) Experimental product currently covering mid 2009 – mid 2010		Merged ensemble product
XCH4_SCI	XCH_4	Level 2, CH_4 column-averaged dry-air mole fraction (in ppb)	SCIAMACHY / ENVISAT	WFMD, IMAP (baseline not yet defined (#))		Note: degradation issues after October 2005 (most severe after mid-2010)
XCH4_GOS_FP	XCH_4	Level 2, CH_4 column-averaged dry-air mole fraction (in ppb)	TANSO / GOSAT	SRFP (RemoTeC)	OCFP (UoL-FP)	"Full Physics" (FP) algorithm product
XCH4_GOS_PR	XCH_4	Level 2, CH_4 column-averaged dry-air mole fraction (in ppb)	TANSO / GOSAT	OCPR (UoL-PR)	SRPR (RemoTeC)	"PRoxy" (PR) algorithm product

Table 1: Overview GHG-CCI ECV Core Algorithm (ECA) products. For details please see **Table 2** and **Table 3**. **(*)** See main text for potential restrictions on alternative algorithms/products and EMMA. **(#)** Evaluation during GHG-CCI Phase 1 revealed some significant differences but if was not possible to clearly identify which algorithm/product is better (please see GHG-CCI Algorithm Selection Report **/GHG-CCI ASR/** and Product Validation and Intercomparison Report **/GHG-CCI PVIRv2/** for details).

2 Instruments

This section provides a brief description of the two core GHG-CCI instruments, SCIAMACHY on ENVISAT and TANSO-FTS onboard GOSAT.

2.1 SCIAMACHY/ENVISAT

The SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY, 2002-2012) was a passive remote sensing spectrometer, which observed backscattered, reflected, transmitted or emitted radiation from the atmosphere and Earth's surface, in the wavelength range between approximately 240 and 2380 nm. SCIAMACHY was part of the scientific payload of the ENVISAT satellite, which was launched on 1st of 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 Earth's surface, where (most of) the sources and sinks of CO_2 and CH_4 are located.

2.2 TANSO/GOSAT

The Japanese Greenhouse gases Observing SATellite (GOSAT) **/Kuze et al., 2009/** was launched on 23rd January 2009 by JAXA, the Japanese Space Agency. GOSAT provides the first dedicated global measurements of total column CO_2 and CH_4 from its Short-Wave-Infrared (SWIR) bands **/Yoshida et al., 2013/**. GOSAT 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 2.0 µm providing sensitivity to near-surface CO_2 and CH_4 concentration variations with the fourth channel operating in the thermal infrared between 5.5 and 14.3 µm providing mid-tropospheric sensitivity **/Saitoh et al., 2009/**.

The measurement strategy of TANSO-FTS is optimised for the characterisation of continental-scale CO_2 and CH_4 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 **/Kuze et al., 2009/**. 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 ~100 km 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 GHG-CCI core (ECA) products

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 present at least two different ECAs (baseline and alternative algorithm) are used for each of the main (core) data products (i.e., XCO_2 and XCH_4 from SCIAMACHY and GOSAT). For details please see GHG-CCI website:
http://www.esa-ghg-cci.org/ -> CRDP (Data) -> GHG-CCI Data Products Main Website

Table 2 provides an overview of the XCO_2 ECAs. **Table 3** shows the corresponding information for XCH_4.

The data products generated with ECAs contain a common set of parameters (described in this document) and algorithm specific parameters (not described in this document but in the corresponding Product User Guides (PUGs)).

XCO_2 Core Product Identifier	Algorithm	Institute	Technique	Reference
CO2_SCI_BESD	BESD: Bremen optimal EStimation DOAS SCIAMACHY XCO_2 algorithm	IUP, Univ. Bremen, Germany	Optimal Estimation	Reuter et al., 2010, 2011
CO2_SCI_WFMD (*)	WFM-DOAS (WFMD): Weighting Function Modified DOAS SCIAMACHY XCO_2 algorithm	IUP, Univ. Bremen, Germany	Least-squares DOAS	Schneising et al., 2011, 2012
CO2_GOS_OCFP	OCFP or UoL-FP: University of Leicester's (OCO-based) GOSAT XCO_2 algorithm	University of Leicester (UoL), UK	Optimal Estimation	Boesch et al., 2006, Connor et al., 2008
CO2_GOS_SRFP	SRFP or RemoTeC: SRON/KIT GOSAT XCO_2 algorithm	SRON, Netherlands, in cooperation with KIT, Germany	Phillips-Tikhonov regularization	Butz et al., 2009, 2010; Guerlet et al., 2013a, 2013b
CO2_EMMA (*)	Ensemble algorithm	Lead: IUP, Univ. Bremen, Germany	Level 2 merging algorithm	Reuter et al., 2013

Table 2: Overview GHG-CCI ECV Core Algorithms (ECAs) for XCO_2. (*) Alternative algorithm/product with potential limitations (see **Sect. 1**).

XCH_4 Core Product Identifier	Algorithm	Institute	Technique	Reference
CH4_SCI_WFMD	WFM-DOAS (WFMD): Weighting Function Modified DOAS SCIAMACHY XCH_4 algorithm	IUP, Univ. Bremen, Germany	Least-squares DOAS; PRoxy (PR) method using CO_2	Schneising et al., 2011, 2012
CH4_SCI_IMAP	IMAP-DOAS (IMAP): Iterative Maximum A Posteriori DOAS SCIAMACHY XCH_4 algorithm	SRON, Netherlands, in cooperation with JPL, USA	Iterative maximum a posteriori DOAS method; PRoxy (PR) method using CO_2	Frankenberg et al., 2005, 2011
CH4_GOS_OCPR	OCPR or UoL-PR: University of Leicester's (OCO-based) GOSAT XCH_4 proxy algorithm	University of Leicester (UoL), UK	Optimal Estimation; PRoxy (PR) method using CO_2	Parker et al., 2011
CH4_GOS_SRFP	SRFP or RemoTeC: SRON/KIT GOSAT XCH_4 full physics algorithm	SRON, Netherlands, in cooperation with KIT, Germany	Phillips-Tikhonov regularization; Full Physics (FP) method	Butz et al., 2009, 2010; Guerlet et al., 2013a
CH4_GOS_OCFP (*)	OCFP or UoL-PR: University of Leicester's (OCO-based) GOSAT XCH_4 full physics algorithm	University of Leicester (UoL), UK	Optimal Estimation; Full Physics (FP) method	Parker et al., 2011
CH4_GOS_SRPR (*)	SRPR or RemoTeC: SRON/KIT GOSAT XCH_4 proxy algorithm	SRON, Netherlands, in cooperation with KIT, Germany	Phillips-Tikhonov regularization; PRoxy (PR) method using CO_2	Butz et al., 2009, 2010

Table 3: Overview GHG-CCI ECV Core Algorithms (ECAs) for XCH_4. (*) Alternative algorithm/product with potential limitations (see **Sect. 1**).

3.1 File format and file naming convention

User requirements for GHG-CCI core products are given in the GHG-CCI URDv1 **/Buchwitz et al., 2011/** and specific data format requirements are given in Data Standards Requirements for CCI Data Producers **/Bennett and James, 2013/**. Both documents have been considered for this version of the PSD.

The required file format is described in **/Bennett and James, 2013/**, requirement R-1:

All CCI projects shall produce data according to the following minimum requirements for data products:
CCI projects shall produce data according to the CCI Data Standards Requirements: • Produced in netCDF-4 (classic) format (see http://www.unidata.ucar.edu/software/netcdf/) • Conform with the CF (Climate and Forecasting) convention 3 (currently version 1.6) • CF standard names used for the main variables • Include the global attributes listed in **/Bennett and James, 2013/**
Note: For netCDF-4 (classic) format, the mode must be set to NC_CLASSIC_MODEL, but compression can be invoked. If netCDF-4 cannot be used (e.g. user tools not yet mature enough), data may be produced in netCDF-3 format.
Files can be checked for compliance with the CF convention using the on-line checking tool : http://cfpcmdi.llnl.gov/conformance/compliance-checker

These requirements have been considered for the products described in this document.

In particular, the netCDF-4 (classic) format is used and the products are in-line with CF (Climate and Forecasting) convention 3.

Concerning the requirement to use CF standard names for the main variables: The process to register "XCO_2" and "XCH_4" as standard names has been initiated (but at the time of writing of this document the registration process was still ongoing). Details on the file content are given in the following sections.

As required **/Bennett and James, 2013/** the following convention is used:

The **directory structure** consists of archive-root (ESACCI/GHG), sensor (satellite or satellite instrument), product (for example BESD_CO2 or SRFP_CH4), version (product version) and time (YYYY, i.e., year only).

Examples:

./ESACCI/GHG/SCIAMACHY/BESD_CO2/v02.00.08/2002/

./ESACCI/GHG/GOSAT/SRFP_CH4/v2.11/2012/

The **file names** consist of ESACCI, CCI project (GHG), processing level (L2), product type (CO2 / CH4), sensor (e.g., SCIAMACHY), algorithm (e.g., BESD or SRFP), date (YYYYMMDD), file version (fv#) and file name extension (.nc), separated by hyphens ("-").

Examples:

ESACCI-GHG-L2-CO2-SCIAMACHY-BESD-20021216-fv1.nc

ESACCI-GHG-L2-CH4-GOSAT-SRFP-20120909-fv1.nc

Each *.nc product file corresponds to one day of satellite observations.

3.2 Common Parameters

The users of the GHG ECV data products, as represented by the GHG-CCI Climate Research Group (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. The GHG-CCI data products are (therefore) Level 2 products. For details please see the GHG-CCI User Guide **/Buchwitz et al., 2011/**).

In order to provide the desired information and to be in agreement with the CCI Data Standard Requirements **/Bennett and James, 2013/** it is required that all ECA products contain at least the parameters listed in the tables below (**Table 4** and **Table 5**).

In order to use our products as easily as possible we have aimed at harmonizing our various products. The goal was to make sure that users can easily switch from one product to another. This has been achieved for all products and parameters with the **exception** of the averaging kernels and related parameters. These parameters are closely related to retrieval algorithm specific characteristics and require special consideration by the users of our products as is explained in detail in **Section 3.3**.

Dimensions in **Table 4** and **Table 5** are defined as follows:

- ***n*:** number of satellite observations (ground pixels) (per file, i.e., for the given day of observations)
- For Averaging Kernel (AK) and related parameters:
    - As explained in **Section 3.3**, the AK and related parameters are provided for “layer-based AKs” and “level-based AKs”
        - For layer-based AK ***m*** is the number of layers which are defined by ***k = m+1*** pressure levels.
        - For level-based AK only levels are used. Here all parameters have the same number of elements, namely ***m*** levels. Here the number of pressure levels is also ***m*** (i.e., ***k = m***).

Table 4 and **Table 5** present an overview about all common parameters including a short description of each parameter. A detailed description is given afterwards.

Name	Type	Dimensions	Units	Short Description
Common parameters for XCO_2 products:				
xco2	Float	n	micromol per mol, abbreviated ppm, i.e., 10^{-6}	Retrieved column-averaged dry-air mole fraction of atmospheric carbon dioxide (XCO_2) in ppm.
xco2_uncertainty	Float	n	micromol per mol, abbreviated ppm, i.e., 10^{-6}	Statistical uncertainty of XCO_2 in ppm (1-sigma).
xco2_averaging_kernel	Float	n x m	[-]	XCO_2 averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XCO_2 retrieval. (see Sect. 3.3)
co2_profile_apriori	Float	n x m	micromol per mol, abbreviated ppm, i.e., 10^{-6}	A priori mole fraction profile of atmospheric CO_2 in ppm. (see Sect. 3.3)
xco2_quality_flag	Byte	n	[-]	Quality flag for XCO_2 retrieval. 0=good.
Common parameters for XCH_4 products:				
xch4	Float	n	nanomol per mol, abbreviated ppb, i.e., 10^{-9}	Retrieved column-averaged dry-air mole fraction of atmospheric methane (XCH_4) in ppb.
xch4_uncertainty	Float	n	nanomol per mol, abbreviated ppb, i.e., 10^{-9}	Statistical uncertainty of XCH_4 in ppb (1-sigma)
xch4_averaging_kernel	Float	n x m	[-]	XCH_4 averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the XCH_4 retrieval. (see Sect. 3.3)
ch4_profile_apriori	Float	n x m	nanomol per mol, abbreviated ppb, i.e., 10^{-9}	A priori mole fraction profile of atmospheric CH_4 in ppb. (see Sect. 3.3)
xch4_quality_flag	Byte	n	[-]	Quality flag for XCH_4 retrieval, 0 = good.
Common parameters for XCO_2 and XCH_4 products: See continuation Table 5				

Table 4: Common parameters for the SCIAMACHY and TANSO XCO_2 and XCH_4 data products generated with ECAs. To be continued via **Table 5**.

Name	Type	Dimensions	Units	Short Description
Common parameters for XCO_2 and XCH_4 products:				
solar_zenith_angle	Float	n	Degrees	Solar zenith angle
sensor_zenith_angle	Float	n	Degrees	Sensor zenith angle
time	Double	n	Seconds	Measurement time
longitude	Float	n	Degrees	Center longitude of the measurement
latitude	Float	n	Degrees	Center latitude of the measurement
pressure_levels	Float	n x k (k = m or k = m+1, see Sect. 3.3)	hPa	Vertical altitude coordinate in pressure units as used for averaging kernels (see Sect. 3.3)
pressure_weight	Float	n x m	[-]	Pressure weights as used for averaging kernels (see Sect. 3.3)

Table 5: Continuation of **Table 4**.

Description of each parameter:

xco2

Main XCO_2 parameter. Retrieved column-average dry-air mole fraction of atmospheric carbon dioxide (XCO_2) in ppm.

xco2_uncertainty

Statistical uncertainty of main XCO_2 parameter: 1-sigma uncertainty of the retrieved XCO_2 in ppm.

xco2_averaging_kernel

XCO_2 averaging kernel (for each observation: vertical profile = vector of dimension *m*).

Represents the sensitivity of the retrieved XCO_2 to atmospheric carbon dioxide mole fraction perturbations depending on pressure (height).

For details please see **Sect. 3.3**.

co2_profile_apriori

A priori mole fraction profile of atmospheric carbon dioxide in ppm needed to apply the XCO_2 averaging kernels.

For details please see **Sect. 3.3**.

xco2_quality_flag

Quality flag for XCO_2 retrieval. 0 = good. 1 = bad.

xch4

Main XCH_4 parameter. Retrieved column-average dry-air mole fraction of atmospheric methane (XCH_4) in ppb

xch4_uncertainty

Statistical uncertainty of main XCH_4 parameter: 1-sigma uncertainty of the retrieved XCH_4 in ppb.

xch4_averaging_kernel

XCH_4 averaging kernel (for each observation: vertical profile = vector of dimension *m*).

Represents the sensitivity of the retrieved XCH_4 to atmospheric methane mole fraction perturbations depending on pressure (height).

For details please see **Sect. 3.3**.

ch4_profile_apriori

A priori mole fraction profile of atmospheric methane in ppb needed to apply the XCH_4 averaging kernels.

For details please see **Sect. 3.3**.

xch4_quality_flag

Quality flag for XCH_4 retrieval. 0 = good. 1 = bad.

solar_zenith_angle

Solar zenith angle (SZA). Angle between the line of sight to the sun and the local vertical. SZA is a positive number (i.e., larger or equal to 0 deg).

sensor_zenith_angle

Sensor zenith angle is the angle between the line of sight from the observed ground pixel to the sensor and the local vertical. The sensor zenith angle is a positive number (i.e., larger or equal to 0 deg; 0 deg for exact nadir (downlooking) observation).

time

Measurement time in seconds since 01.01.1970 00:00:00.

longitude

Center longitude of the measurement. A number in the range -180 deg to +180 deg.
0 deg passes through Greenwich.

latitude

Center latitude of the measurement. A number in the range -90 deg (south pole) to +90 deg (north pole). 0 deg = equator.

pressure_levels

Pressure levels as used for the averaging kernels. Ordered from the bottom of the atmosphere to the top of the atmosphere (i.e., by decreasing pressure).

For details please see **Sect. 3.3**.

pressure_weight

Layer / level dependent weights needed to apply the averaging kernels.

For details please see **Sect. 3.3**.

3.3 How to use the Averaging Kernels (AKs)?

3.3.1 Introduction

In order to compare the satellite-retrieved XCO_2 and XCH_4 data products with model simulations and for inverse modelling of surface fluxes (see, e.g., **/Bergamaschi el al., 2007/**) the altitude sensitivity of the satellite retrievals has to be taken into account. Information on the altitude sensitivity is provided by the satellite XCO_2 and XCH_4 averaging kernels and corresponding CO_2 and CH_4 *a priori* vertical profiles.

Also for validation purposes the averaging kernels have to be considered, see, e.g., **/Wunch et al., 2010, 2011/**, **/Dils et al., 2013/** and TCCON website (in particular https://tccon-wiki.caltech.edu/Network_Policy/Data_Use_Policy/Auxiliary_Data).

All common variables described in the previous section (e.g., xco2, xco2_uncertainty, time, longitude, etc.) can be used identically for all GHG-CCI ECA products with the **exception** of the averaging kernels and related parameters, as these parameters are closely related to the retrieval algorithm used.

In this section it is explained how the averaging kernels and related parameters can be used.

How these parameters have been defined depends on the retrieval algorithm used to generate a certain product and it was not possible to fully harmonize their use, i.e., their use depends on the product.

The purpose of this section is to explain how to use the averaging kernels and their related parameters and for which data product which method is recommended.

There are two different averaging kernel (AK) categories:
Depending on product, the AKs are

- "layer-based" (IUP, Univ. Bremen, and SRON products)

or

- "level-based" (Univ. Leicester products).

In the following sub-sections more information on this is given including the information for which product which category is valid.

Note that user can also determine "automatically" or via inspection of the product files which category a given product belongs to:

- For "layer-based" products the vertical dimension of parameter **pressure_levels** is *m+1*, i.e., there is one entry more than for parameter **pressure_weight** (or any of the other parameters with a vertical dimension), which has *m* vertical entries, i.e., one entry less than parameter **pressure_levels**.
- For "level-based" products all parameters have *m* entries.

In the following sub-sections the relevant parameters are listed and shortly explained (**Sect. 3.3.2**) followed by detailed explanations of how these parameters can be used for the layer-based AK products (**Sect. 3.3.3**) and for the level-based AK products (**Sect. 3.3.4**).

Important note:
The AK related parameters and how they can be used as described in this document is most interesting for users who want to use different products and prefer to easily switch from one product to another. The main purpose of the common parameters and methods described in this document is to provide the users with the parameters and formulas to do this. However, all products also contain additional parameters, not described in this document, but in the PUGs of the individual products (please see also the Algorithm Theoretical Basis Documents (ATBDs) of the individual algorithms used to generate the individual products). Using these additional parameters (and corresponding formulas) users may be able to obtain somewhat more accurate results (although the differences are expected to be very small).

3.3.2 Averaging kernel (AK) related parameters

For each single observation (ground pixel) several averaging kernel related parameters are contained in the satellite product files. These parameters are listed in **Table 6**.

For additional information and how to use these parameters see the following two sub-sections.

Parameter Name	Mathematical symbol	Dimension (*)	Unit	Explanation
pressure_levels	*p*	*k*	[hPa]	Pressure levels; note: *k = m +1* (for layer-based approach) or *k = m* (for level-based approach)
pressure_weight	*pw*	*m*	[-]	Pressure weights for all layers / levels
xco2_averaging_kernel	*AK*	*m*	[-]	XCO_2 averaging kernel
co2_profile_apriori	*VMR*	*m*	µmol/mol, abbreviated ppm (10^{-6})	CO_2 *a priori* profile
xch4_averaging_kernel	*AK*	*m*	[-]	XCH_4 averaging kernel
ch4_profile_apriori	*VMR*	*m*	nanomol/mol, abbreviated ppb (10^{-9})	CH_4 *a priori* profile

Table 6: Overview of averaging kernel (AK) and related parameters. (*) Here the ground pixel dimension (n, see previous sections, **Table 4** and **Table 5**) is not shown, i.e., here each array is 1-dimensional (a vector). Each element corresponds to one atmospheric level or layer as explained in the following sections.

3.3.3 How to use layer-based AKs?

In this section it is described how the common parameters related to averaging kernels (AKs) can be used to apply the satellite's AKs to model profiles in order to take the altitude sensitivity of the satellite's XCO_2 and XCH_4 retrievals into account.

As indicated at the end of **Sect. 3.3.1**, each product may (or may not) contain additional parameters and corresponding formulas, not described in this document (but in the corresponding PUG), which can be used to obtain somewhat more accurate results for a specific product (although the differences compared to the method described in this section are expected to be small).

For the layer-based approach the AKs and corresponding *a priori* CO_2 and CH_4 profiles are defined for layers and they correspond to layer averages. There are ***m*** layers, which are defined by ***k = m+1*** pressure levels.

The "AK layer-based approach", which is explained in this sub-section, needs to be applied for the following GHG-CCI ECA products (all IUP, Univ. Bremen, and SRON products):

- CO2_SCI_BESD
- CO2_GOS_SRFP
- CO2_EMMA
- CH4_SCI_WFMD
- CH4_SCI_IMAP
- CH4_GOS_SRFP
- CH4_GOS_SRPR

As already described above:
Note that user can also determine "automatically" or via inspection of the product files which category a given product belongs to:

- For "layer-based" products the vertical dimension of parameter **pressure_levels** is *m+1*, i.e., there is one entry more than for parameter **pressure_weight** (or any of the other parameters with a vertical dimension), which has *m* vertical entries, i.e., one entry less than parameter **pressure_levels**.
- For "level-based" products all parameters have *m* entries.

The layer-based approach is also described and used in **/Bergamaschi et al., 2007/**. Here a slightly modified version of their Eq. 2 is shown (here GHG = CO_2 or CH_4):

$$XGHG^{mod} = \sum_{i=1}^{m}\left[VMR_i^{apri} + AK_i(VMR_i^{mod} - VMR_i^{apri})\right] pw_i \qquad \textbf{Eq. (1)}$$

- Here $XGHG^{mod}$ is the desired modelled XCO_2 or XCH_4 value, which corresponds to the satellite XCO_2 or XCH_4 retrievals.
- The sum is over the m atmospheric layers (located between pressure levels p_i and p_{i+1} with $i = 1...m$). Here pressure is the "normal" or "total" or "wet" pressure (not the "dry pressure", see below). Here $i = 1$ corresponds to the bottom of the atmosphere and $i = k = m+1$ corresponds to the top of the atmosphere.

- pw_i is a layer-dependent weight (depending on algorithm/product this corresponds to $\Delta p_i/p_{surf}$ of **/Bergamaschi et al., 2007/** times a conversion factor for the conversion of wet to dry pressure).
- VMR_i^{apri} is the satellite *a priori* layer-averaged CO_2 or CH_4 volume mixing ratio (VMR) or, more precisely, Dry Mole Fraction (DMF), between pressure levels $p_i$and p_{i+1}(note: $p_i > p_{i+1}$).
- VMR_i^{mod} is the corresponding value of the model (CO_2 of CH_4) VMR (DMF) between pressure levels p_i and p_{i+1}.
- AK_i is the satellite XCO_2 or XCH_4 averaging kernel for layer i.

Note that in this equation all parameters are coming from the satellite product with the exception of VMR_i^{mod}.

Note that the described approach permits to use all satellite data as they are without the need to manipulate them, e.g., by interpolation. Only the model quantity VMR_i^{mod} needs to be computed.

For illustration and a short overview please see **Figure 1**.

For a modeler the receipt to compute $XGHG^{mod}$ is the following:

- For each satellite observation:
  - Interpolate the model profiles to the location and time of the satellite observation.
  - Compute for each satellite layer i, as defined by pressure levels p_i and p_{i+1}:
    - The layer-averaged model (CO_2 or CH_4) VMR (DMF), i.e., VMR_i^{mod}
  - Apply the formula given above to compute the desired quantity $XGHG^{mod}$ (see also **Figure 1** and **Figure 2**).

Figure 1 and **Figure 2** explain how the parameters as provided via the satellite product files (**Table 6**) have to be used in order to apply **Eq. (1)**.

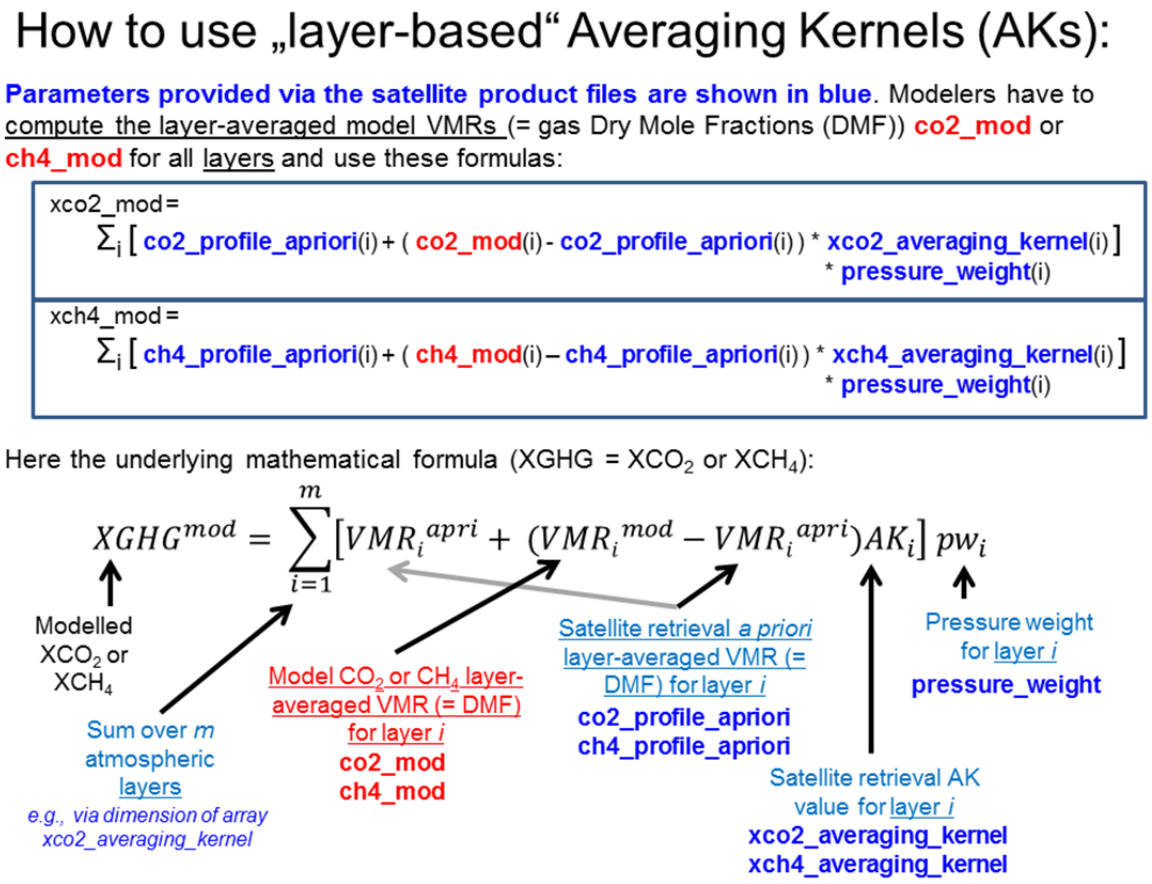

Figure 1: Overview how to compute XCO_2 or XCH_4 (= XGHG) using the „layer-based“ AK method. Additional explanations are given in **Figure 2**.

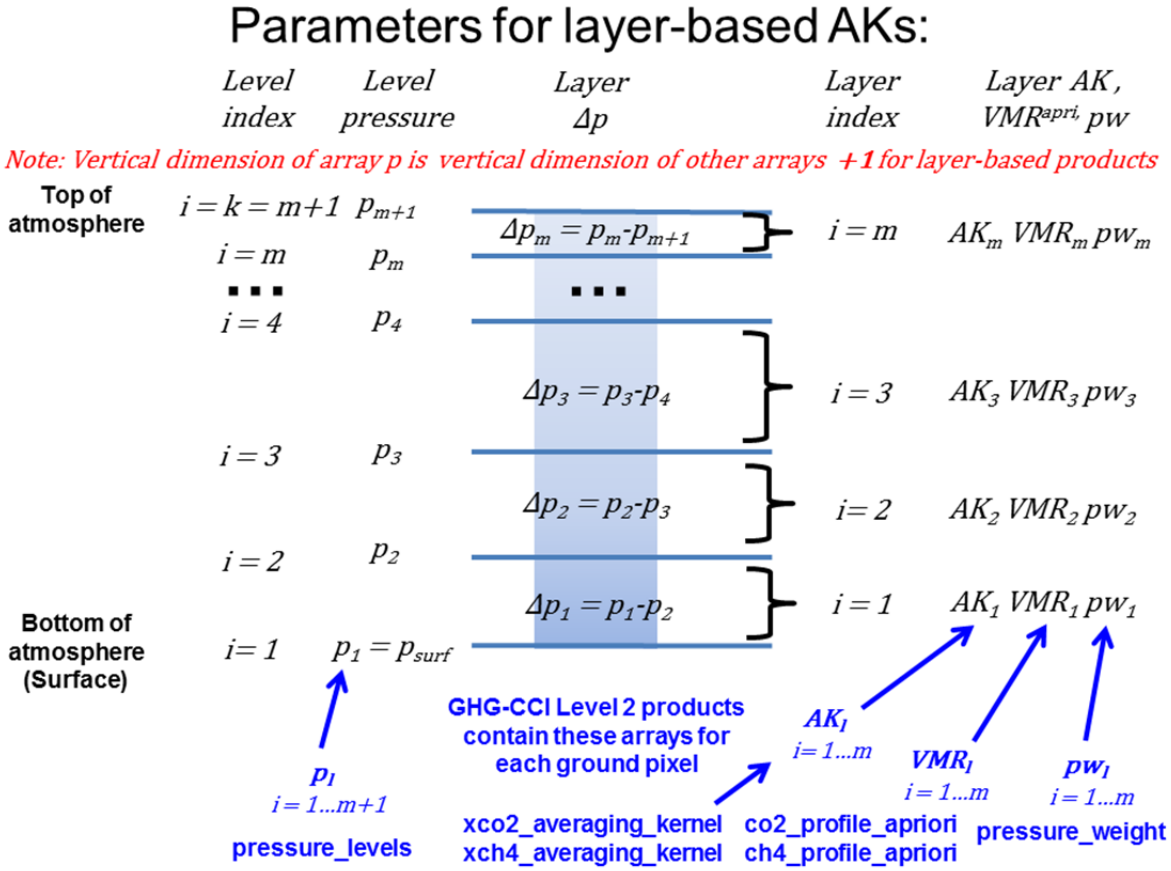

Figure 2: Additional explanations related to the parameters needed to use the "layer-based AK approach" (see also **Figure 1**).

3.3.4 How to use level-based AKs?

For the level-based approach the AKs and corresponding *a priori* VMR (= DMF) profiles are defined on levels (not on layers).

The same parameters (variable names etc.) as provided via the satellite products files are used as for the layer-based approach described in the previous section but with a slightly different implementation to apply these parameters to compute the modelled XCO_2 or XCH_4.

For the level-based approach all AK related arrays are given for *m* levels.

The "AK level-based approach", which is explained in this sub-section, needs to be applied for the following GHG-CCI ECA products (all UoL products, i.e., all "OC" products):

- CO2_GOS_OCFP
- CH4_GOS_OCPR
- CH4_GOS_OCFP

As already described above:
Note that user can also determine "automatically" or via inspection of the product files which category a given product belongs to:

- For "layer-based" products the vertical dimension of parameter **pressure_levels** is *m+1*, i.e., there is one entry more than for parameter **pressure_weight** (or any of the other parameters with a vertical dimension), which has *m* vertical entries, i.e., one entry less than parameter **pressure_levels**.
- For "level-based" products all parameters have *m* entries.

For model comparisons and inverse modelling the following method is recommended in order to compute the modelled XCO_2 or XCH_4.

The equation to apply the level-based averaging kernels to the model data is the same as for the layer-based approach (**Eq. 1**) but with the variables now all on levels, rather than layers. The key point is that the model data (co2_mod or ch4_mod in **Fig. 3**) must be interpolated onto the retrieval pressure levels (p_i). This interpolation should be done with care so as to conserve the total column amounts of $XGHG$.

For illustration and a short overview please see **Figure 13**.

For a modeler the recipe to compute $XGHG^{mod}$ is the following:

- For each satellite observation:
  - Interpolate the model profiles to the location and time of the satellite observation.
  - Compute for model data at each satellite retrieval pressure level i the model VMR, i.e., VMR_i^{mod}
  - Apply the formula given above (**Eq. (1)**) to compute the desired quantity $XGHG^{mod}$ (see also **Figure 13** and **Figure 24**).

Figure 13 and **Figure 2**4 explain how the parameters as provided via the satellite product files (**Table 6**) have to be used in order to apply **Eq. (1)**.

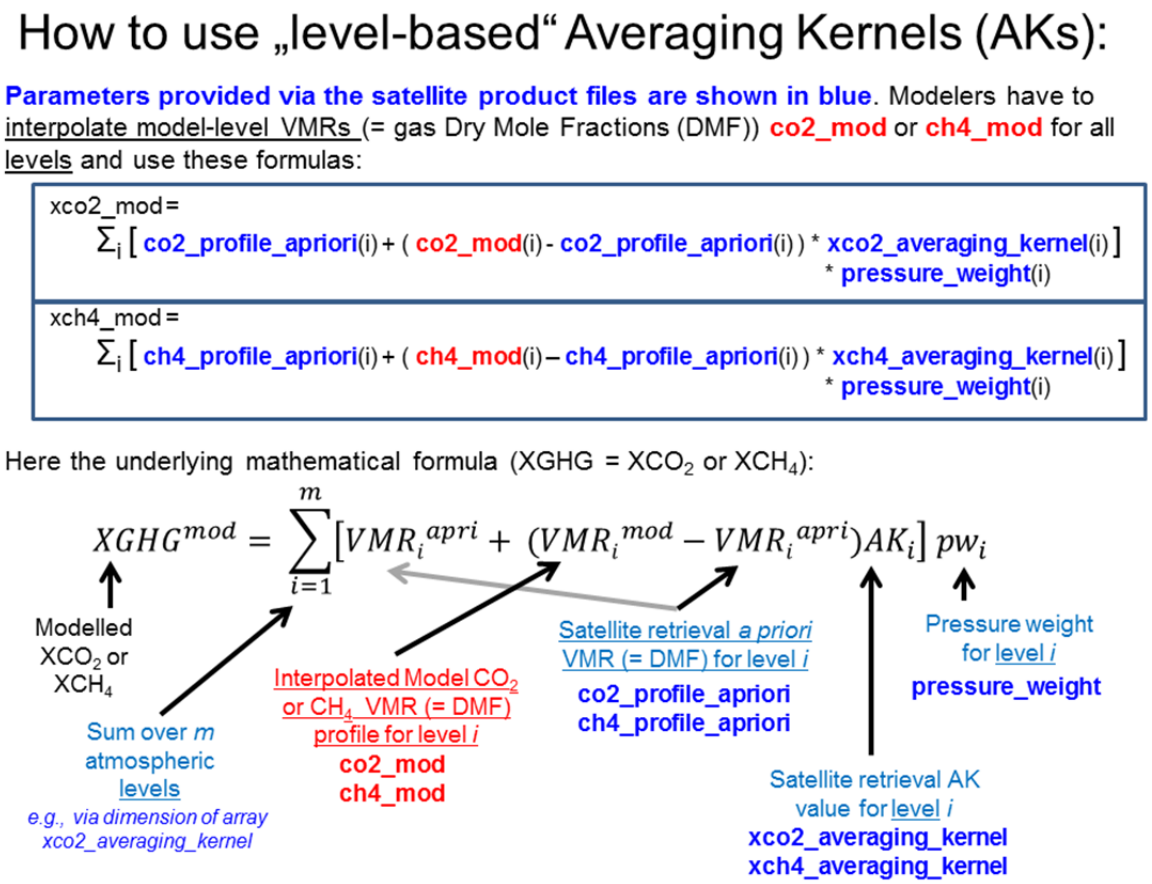

Figure 3: Overview how to compute XCO_2 or XCH_4 (= XGHG) using the „level-based“ AK method. Additional explanations are given in **Figure 4**.

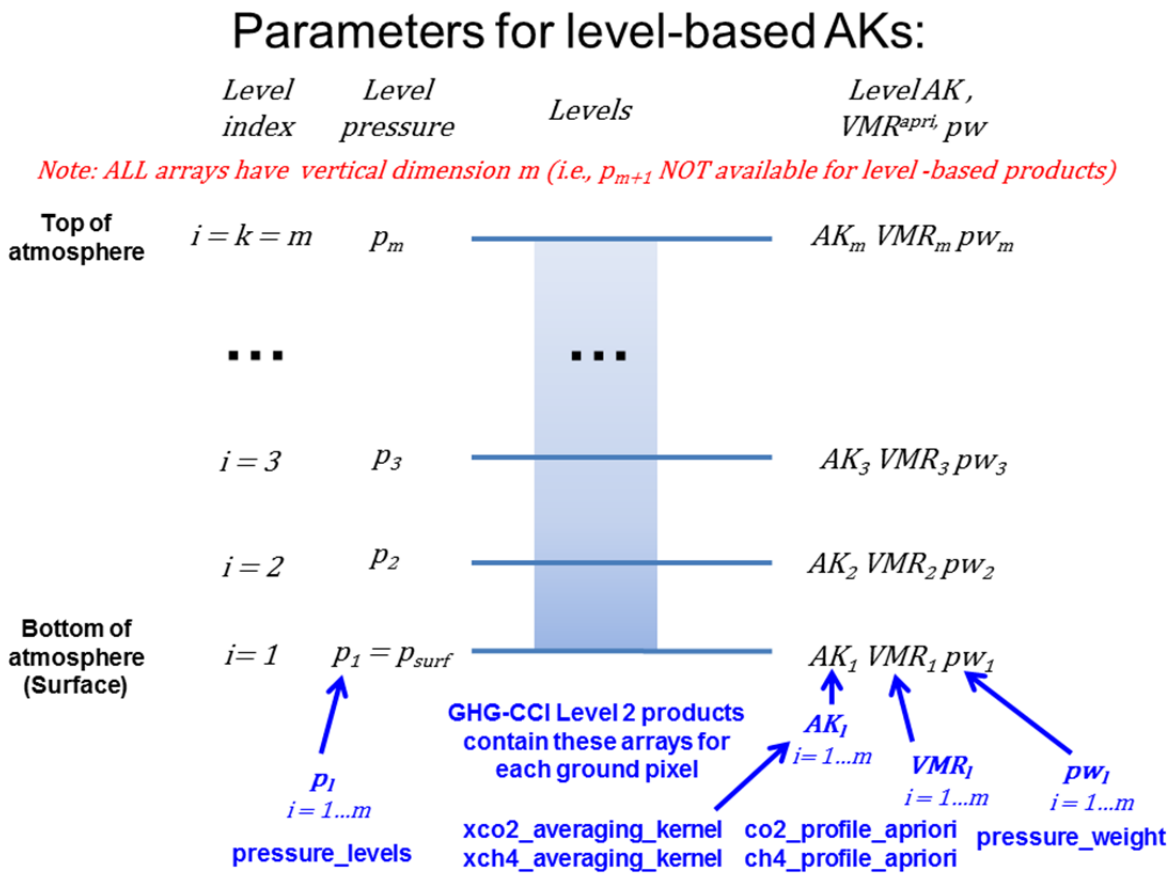

Figure 4: Additional explanations related to the parameters needed to use the "level-based AK approach" (see also **Figure 3**).

3.4 Algorithm-Specific Parameters

In addition to the common parameters listed above, a full description of all algorithm-specific parameters is provided in the Product User Guide (PUG) of each product.

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5 Acronyms

Abbreviation	Meaning
ACA	Additional Constraints Algorithm (of GHG-CCI)
AK	Averaging Kernel
ASR	Algorithm Selection Report
ATBD	Algorithm Theoretical Basis Document
BESD	Bremen optimal EStimation DOAS
CCI	Climate Change Initiative
CRDP	Climate Research Data Package
DMF	Dry Mole Fraction
DOAS	Differential Optical Absorption Spectroscopy
ECA	ECV Core Algorithm (of GHG-CCI)
ECV	Essential Climate Variable
EMMA	Ensemble Median Algorithm
ESA	European Space Agency
FCDR	Fundamental Climate Data Record
FP	Full Physics
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
GMES	Global Monitoring for Environment and Security
GOSAT	Greenhouse Gas Observing Satellite
IMAP-DOAS	Iterative Maximum A posteriori (IMAP) DOAS

IPCC	International Panel in Climate Change
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
MACC	Monitoring Atmospheric Composition and Climate, EU GMES project
MIPAS	Michelson Interferometer for Passive Atmospheric Sounding
NASA	National Aeronautics and Space Administration
NIES	National Institute for Environmental Studies
NOAA	National Oceanic and Atmospheric Administration
OCO	Orbiting Carbon Observatory
OE	Optimal Estimation
PBL	Planetary Boundary Layer
PR	PRoxy algorithm
PUG	Product User Guide
PVIR	Product Validation and Intercomparison Report
RTM	Radiative transfer model
SCIATRAN	Radiative transfer model for SCIAMACHY developed and continuously improved at IUP
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric CHartograghY
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
VMR	Volume Mixing Ratio
WFM-DOAS (or WFMD)	Weighting Function Modified DOAS

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