



Algorithm Theoretical Basis Document (ATBD) – ANNEX D for products XCO2_EMMA and XCH4_EMMA (v3.1, 2003-2017)

C3S_312a_Lot6_IUP-UB – Greenhouse Gases

Issued by: Maximilian Reuter, University of Bremen,

Institute of Environmental Physics (IUP)

Date: 04/10/2018

Ref: C3S_D312a_Lot6.2.1.2-v2_ATBD_ANNEX-D_v2.0

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



This document has been produced in the context of the Copernicus Climate Change Service (C3S).

The activities leading to these results have been contracted by the European Centre for Medium-Range Weather Forecasts, operator of C3S on behalf of the European Union (Delegation Agreement signed on 11/11/2014). All information in this document is provided "as is" and no guarantee or warranty is given that the information is fit for any particular purpose.

The user thereof uses the information at its sole risk and liability. For the avoidance of all doubts, the European Commission and the European Centre for Medium-Range Weather Forecasts has no liability in respect of this document, which is merely representing the authors view.



Contributors

**INSTITUTE OF ENVIRONMENTAL PHYSICS (IUP),
UNIVERSITY OF BREMEN, BREMEN, GERMANY
(IUP)**

M. Reuter

M. Buchwitz

O. Schneising-Weigel



Table of Contents

History of modifications	5
Related documents	6
Acronyms	7
General definitions	11
Scope of document	12
Executive summary	13
Data product overview	14
Input and auxiliary data	20
1.1 Satellite instrument	20
1.2 Other	20
Algorithms	22
1.3 Ensemble spread	22
1.4 Ensemble median	26
Output data	28
References	30



History of modifications

Version	Date	Description of modification	Chapters / Sections
1.1	20-October-2017	New document for data set CDR1 (2003-2016)	All
2.0	4-October-2018	Update for CDR2 (2003-2017)	All



Related documents

Reference ID	Document
D1	Main ATBD: Buchwitz, M., et al., Algorithm Theoretical Basis Document (ATBD) – Main document, C3S project C3S_312a_Lot6_IUP-UB – Greenhouse Gases, v2.0, 2018. <i>(this document is an ANNEX to the Main ATBD)</i>



Acronyms

Acronym	Definition
AIRS	Atmospheric Infrared Sounder
AMSU	Advanced Microwave Sounding Unit
ATBD	Algorithm Theoretical Basis Document
BESD	Bremen optimal EStimation DOAS
CAR	Climate Assessment Report
C3S	Copernicus Climate Change Service
CCDAS	Carbon Cycle Data Assimilation System
CCI	Climate Change Initiative
CDR	Climate Data Record
CDS	(Copernicus) Climate Data Store
CMUG	Climate Modelling User Group (of ESA's CCI)
CRG	Climate Research Group
D/B	Data base
DOAS	Differential Optical Absorption Spectroscopy
EC	European Commission
ECMWF	European Centre for Medium Range Weather Forecasting
ECV	Essential Climate Variable
EMMA	Ensemble Median Algorithm
ENVISAT	Environmental Satellite (of ESA)
EO	Earth Observation
ESA	European Space Agency
EU	European Union
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
FCDR	Fundamental Climate Data Record



FoM	Figure of Merit
FP	Full Physics retrieval method
FTIR	Fourier Transform InfraRed
FTS	Fourier Transform Spectrometer
GCOS	Global Climate Observing System
GEO	Group on Earth Observation
GEOSS	Global Earth Observation System of Systems
GHG	GreenHouse Gas
GOME	Global Ozone Monitoring Experiment
GMES	Global Monitoring for Environment and Security
GOSAT	Greenhouse Gases Observing Satellite
IASI	Infrared Atmospheric Sounding Interferometer
IMAP-DOAS (or IMAP)	Iterative Maximum A posteriori DOAS
IPCC	International Panel in Climate Change
IUP	Institute of Environmental Physics (IUP) of the University of Bremen, Germany
JAXA	Japan Aerospace Exploration Agency
JCGM	Joint Committee for Guides in Metrology
L1	Level 1
L2	Level 2
L3	Level 3
L4	Level 4
LMD	Laboratoire de Météorologie Dynamique
MACC	Monitoring Atmospheric Composition and Climate, EU GMES project
NA	Not applicable
NASA	National Aeronautics and Space Administration
NetCDF	Network Common Data Format
NDACC	Network for the Detection of Atmospheric Composition Change
NIES	National Institute for Environmental Studies
NIR	Near Infra Red



NLIS	LMD/CNRS <i>neuronal</i> network mid/upper tropospheric CO ₂ and CH ₄ retrieval algorithm
NOAA	National Oceanic and Atmospheric Administration
Obs4MIPs	Observations for Climate Model Intercomparisons
OCO	Orbiting Carbon Observatory
OE	Optimal Estimation
PBL	Planetary Boundary Layer
ppb	Parts per billion
ppm	Parts per million
PR	(light path) PROxy retrieval method
PVIR	Product Validation and Intercomparison Report
QA	Quality Assurance
QC	Quality Control
REQ	Requirement
RMS	Root-Mean-Square
RTM	Radiative transfer model
SCIAMACHY	SCanning Imaging Absorption spectroMeter for Atmospheric ChartographY
SCIATRAN	SCIAMACHY radiative transfer model
SRON	SRON Netherlands Institute for Space Research
SWIR	Short Wave Infra Red
TANSO	Thermal And Near infrared Sensor for carbon Observation
TANSO-FTS	Fourier Transform Spectrometer on GOSAT
TBC	To be confirmed
TBD	To be defined / to be determined
TCCON	Total Carbon Column Observing Network
TIR	Thermal Infra Red
TR	Target Requirements
TRD	Target Requirements Document
WFM-DOAS (or WFMD)	Weighting Function Modified DOAS
UoL	University of Leicester, United Kingdom



URD	User Requirements Document
WMO	World Meteorological Organization
Y2Y	Year-to-year (bias variability)



General definitions

Table 1 lists some general definitions relevant for this document.

Table 1: General definitions.

Item	Definition
XCO ₂	Column-averaged dry-air mixing ratios (mole fractions) of CO ₂
XCH ₄	Column-averaged dry-air mixing ratios (mole fractions) of CH ₄
L1	Level 1 satellite data product: geolocated radiance (spectra)
L2	Level 2 satellite-derived data product: Here: XCO ₂ and XCH ₄ information for each ground-pixel
L3	Level 3 satellite-derived data product: Here: Gridded XCO ₂ and XCH ₄ information, e.g., 5°x5°, monthly
L4	Level 4 satellite-derived data product: Here: Surface fluxes (emission and/or uptake) of CO ₂ and CH ₄



Scope of document

This document is an Algorithm Theoretical Basis Document (ATBD) for the Copernicus Climate Change Service (C3S, <https://climate.copernicus.eu/>) component as covered by project C3S_312a_Lot6 led by University of Bremen, Germany.

Within project C3S_312a_Lot6 satellite-derived atmospheric carbon dioxide (CO₂) and methane (CH₄) Essential Climate Variable (ECV) data products will be generated and delivered to ECMWF for inclusion into the Copernicus Climate Data Store (CDS) from which users can access these data products and the corresponding documentation.

The C3S_312a_Lot 6 satellite-derived data products are:

- Column-averaged dry-air mixing ratios (mole fractions) of CO₂ and CH₄, denoted XCO₂ (in parts per million, ppm) and XCH₄ (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of CO₂ (in ppm) and CH₄ (in ppb).

This document describes the algorithms to generate the C3S products XCO₂_EMMA and XCH₄_EMMA.

These products are merged multi-sensor XCO₂ and XCH₄ Level 2 products generated using algorithms developed at University of Bremen, Germany.



Executive summary

This ATBD describes the algorithm theoretical basis for EMMA v3.1 CO₂ and EMMA v3.1 CH₄. Originally, the EMMA algorithm (v1.3) was described in detail at the example of CO₂ in the publication of *Reuter et al. (2013)* and their publication is the blueprint for this ATBD.

Since long time, climate modelers use ensemble approaches to calculate the ensemble median and to estimate uncertainties of climate projections where no ground-truth is known. Following this idea, the ensemble median algorithm EMMA composes level 2 data of several GOSAT and SCIAMACHY XCO₂ and XCH₄ retrieval products independently developed by NASA, NIES, SRON, University of Leicester, and the University of Bremen. EMMA determines in 10°x10° degree grid boxes monthly averages and selects the level 2 data of the median algorithm. Thresholds depending on potential information content prevent from over-weighting individual algorithms with a considerably larger amount of data.

The EMMA database consists of individual level 2 soundings retrieved by algorithms which can change from grid box to grid box and month to month. Therefore, it can be used in the same manner as any other XCO₂ or XCH₄ satellite retrieval, i.e., the EMMA database includes all information needed for inverse modeling (geo-location, time, XCO₂ or XCH₄, averaging kernels, etc.). Additionally, it includes the inter-algorithm spread which informs about potential regional uncertainties.



Data product overview

Our current knowledge about the sources and sinks of atmospheric CO₂ and CH₄ is limited by the sparseness of highly accurate and precise measurements of these gases (e.g., *Stephens et al., 2007*). Due to their global coverage and sensitivity down to the surface, satellite based XCO₂ and XCH₄ (column-average dry-air mole fraction of atmospheric CO₂ and CH₄) retrievals in the near infrared are promising candidates to reduce existing uncertainties if accurate and precise enough (e.g., *Rayner and O'Brien, 2001; Houweling et al., 2004; Miller et al., 2007; Chevallier et al., 2007*).

At present, several independently developed XCO₂ and XCH₄ retrieval algorithms exist for SCIAMACHY (scanning imaging absorption spectrometer of atmospheric chartography; *Burrows et al., 1995; Bovensmann et al., 1999*) and GOSAT (greenhouse gases observing satellite; *Yokota et al., 2004*); see **Table 2** and **Table 3** for those used for EMMA v3.1 CO₂ and EMMA v3.1 CH₄, respectively.

All retrieval teams find encouraging validation results when comparing with TCCON (total carbon column observing network, *Wunch et al., 2011*) ground based FTS (Fourier transform spectrometer) measurements (see references in the next section). This goes along with a good inter-algorithm agreement at TCCON sites and with the results of our unified validation study having station-to-station biases (i.e., the standard deviation of the biases at different sites) usually below 0.6ppm and 5.0ppb and single measurement precisions usually below 2.0ppm and 15ppb for CO₂ and CH₄, respectively (**Figure 1, Table 4, Figure 2, Table 5**).

However, the inter-algorithm agreement often reduces remote from validation sites due to differing large scale bias patterns (see Sec. 3.1). Such biases can be a critical issue for surface flux inversions and the user requirements are demanding; as an example, *Miller et al. (2007)* and *Chevallier et al. (2007)* found that regional biases of a few tenths of a ppm can already hamper surface flux inversions. This indicates that assessing an algorithm's quality should not be based on comparisons against current TCCON stations only. Obviously, large regions of the world possess more "complicated" retrieval conditions without the availability of ground truth measurements which could be used to judge the algorithms' performance.

Diverging model results are common to many scientific disciplines (e.g., *Araujo and New, 2007; Rötter et al., 2011*) and much attention and effort is devoted to this topic on the subject of weather and climate modeling. Here, the divergence of the model results arises not only from structural differences of the different models, but also from the nonlinearity of the model equations, leading to differing results of one single model when performing multiple realizations with slightly differing initial conditions (*Hagedorn et al., 2005; Tebaldi and Knutti, 2007*).

Especially in the case of weather forecasting or climate projections, where no ground truth is available for the verification of the forecasts and projections, it is impossible to identify the "best" model and the "perfect" initial conditions. For long-term climate projections, this problem is impaired by the unknown future greenhouse forcing.



Table 2: Main retrieval characteristics of EMMA v3.1 CO₂ algorithms: algorithm name and version, satellite instrument, spectral bands, inversion technique (OE = optimal estimation, TP = Tikhonov–Phillips regularization, LS = least squares), consideration of scattering (FP = full physics, PR = light path proxy, xEP20 = x extinction profiles with 20 layers (two aerosol types, water and ice cloud), CWP = cloud water path, CTH = cloud top height, AOD = aerosol optical depth, APNC = aerosol particle number concentration, ASP = aerosol size parameter, AH = aerosol height), main cloud filter (MERIS = medium resolution imaging spectrometer, CAI = cloud and aerosol imager of GOSAT, PMD = polarization measurement device of SCIAMACHY).

Algorithm	Sensor	Bands [μm]				Inversion	Scattering	Primary cloud filter	Empirical bias correction
		0.76	1.58	1.60	2.05				
BESD v02.01.02	SCIAMACHY	•	•			OE	FP (CWP, CTH, APS1)	MERIS	•
RemoTeC v2.3.8	GOSAT	•		•	•	TP	FP (APNC, ASP, AH)	CAI	•
ACOS v7.3.10a	GOSAT	•		•	•	OE	FP (4EP20)	O ₂ -A	•
UoL-FP v7.2	GOSAT	•		•	•	OE	FP (3EP20)	O ₂ -A	•
NIES v02bc	GOSAT	•		•	•	OE	FP (AOD)	CAI	•
PPDF-s v02	GOSAT	•		•	•	OE	PPDF parameters	CAI	
NIES v02	GOSAT	•		•	•	OE	FP (AOD)	CAI	

Table 3: Same as Table 2 but for EMMA v3.1 CH₄ algorithms.

Algorithm	Sensor	Bands [μm]				Inversion	Scattering	Primary cloud filter	Empirical bias correction
		0.76	1.58	1.60	2.05				
WFMD v4.0	SCIAMACHY	•	•			LS	PR (CH ₄ /CO ₂)	PMD	•
RemoTeC-FP v2.3.8	GOSAT	•		•	•	TP	FP (APNC, ASP, AH)	CAI	•
RemoTeC-PR v2.3.9	GOSAT	•		•	•	TP	PR (CH ₄ /CO ₂)	CAI	•
UoL-FP v7.2	GOSAT	•		•	•	OE	FP (3EP20)	O ₂ -A	•
UoL-PR v7.2	GOSAT	•		•	•	OE	PR (CH ₄ /CO ₂)	O ₂ -A	•
NIES v02bc	GOSAT	•		•	•	OE	FP (AOD)	CAI	•
PPDF-S v02	GOSAT	•		•	•	OE	FP (AOD)	CAI	
NIES v02	GOSAT	•		•	•	OE	FP (AOD)	CAI	



Table 4: XCO₂ TCCON validation statistics for the period and sites shown in **Figure 1** with number of co-locations (#), average single measurement precision (σ) relative to TCCON and reported in brackets, and standard deviation of station-to-station biases (Δ).

Algorithm	#	σ [ppm]	Δ [ppm]
BESD v02.01.02	18585	1.84 (1.92)	0.29
RemoTeC v2.3.8	12587	2.13 (2.17)	0.60
ACOS v7.3.10a	11985	1.74 (1.27)	0.58
UoL-FP v7.2	11974	1.80 (1.94)	0.43
NIES v02bc	8952	2.26 (0.95)	0.63
PPDF-S v02	8469	1.95 (0.76)	0.94
NIES v02	14654	2.30 (0.97)	0.67
EMMA v3.1 CO ₂	15743	1.92 (1.92)	0.50

Table 5: Same as **Table 4** but for XCH₄.

Algorithm	#	σ [ppm]	Δ [ppm]
WFMD v4.0	13358	100.54 (88.41)	8.38
RemoTeC-FP v2.3.8	11288	13.98 (13.53)	4.58
RemoTeC-PR v2.3.9	35293	14.26 (12.58)	3.29
UoL-FP v7.2	10942	13.38 (14.53)	3.36
UoL-PR v7.2	30592	13.68 (11.35)	4.42
NIES v02bc	8046	14.04 (6.72)	3.90
PPDF-S v02	7512	14.40 (5.11)	6.66
NIES v02	13802	13.95 (6.91)	4.08
EMMA v3.1 CH ₄	20881	13.68 (13.25)	3.70

This conceptual problem is dealt with by using multi-model, multi-realization, multi-emission-scenario ensembles of simulations, which ideally span the entire range of possible model outcomes and, thus, can be used to estimate the uncertainties of the forecast or projection.

However, interpreting the ensemble's spread as uncertainty is not the only possible application: some studies indicate that the ensemble mean, weighted mean, or median can outperform each



individual model under appropriate conditions (e.g., *Kharin and Zwiers, 2002; Vautard et al., 2009*). Here, we seize this idea and introduce the ensemble median algorithm EMMA which uses data from the retrieval algorithms listed in the next section. EMMA generates a database of individual level 2 retrievals and takes advantage of the variety of different retrieval algorithms and their independent developments.

For each month and each $10^{\circ}\times 10^{\circ}$ grid box, one algorithm is chosen to supply level 2 retrievals for the database. The algorithm is chosen on the basis that its grid box mean is the median amongst the available algorithms. This allows the reduction of occasional outliers and sometimes unrealistic bias patterns, which may be found in each individual retrieval algorithm and which may hamper surface flux inversions. EMMA relies on the assumption that it is unlikely that the majority of algorithms produce outliers in the same direction because only in this case the median is a bad choice.

Smoothing of real atmospheric variability, as it could happen when dealing with climate model ensembles, cannot be expected for EMMA because all ensemble members (XCO₂ or XCH₄ retrieval algorithms) represent the same (real) atmospheric XCO₂ or XCH₄ conditions and deviations from the real values are always due to retrieval errors (sampling issues are neglected in this context).

The EMMA database includes all information needed for inverse modeling (geo-location, time, XCO₂ or XCH₄, averaging kernels, etc.). As it consists of individual XCO₂ or XCH₄ retrievals, it can be used in the same manner as any other XCO₂ or XCH₄ satellite retrieval. Additionally, the EMMA database includes the inter-algorithm spread which gives important information about regional uncertainties.

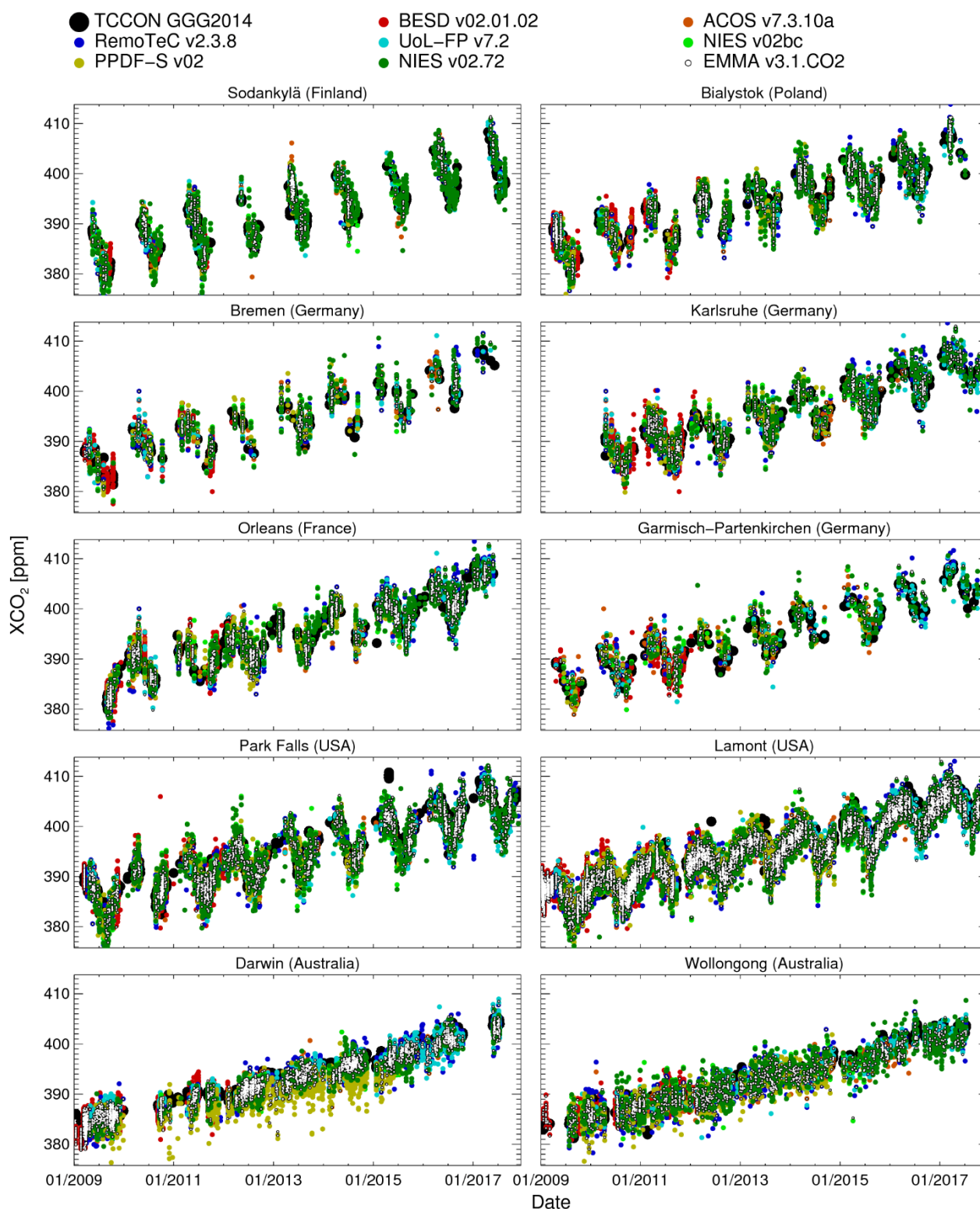


Figure 1: Validation of individual XCO₂ algorithms and EMMA v3.1 CO₂ with TCCON GGG2014.

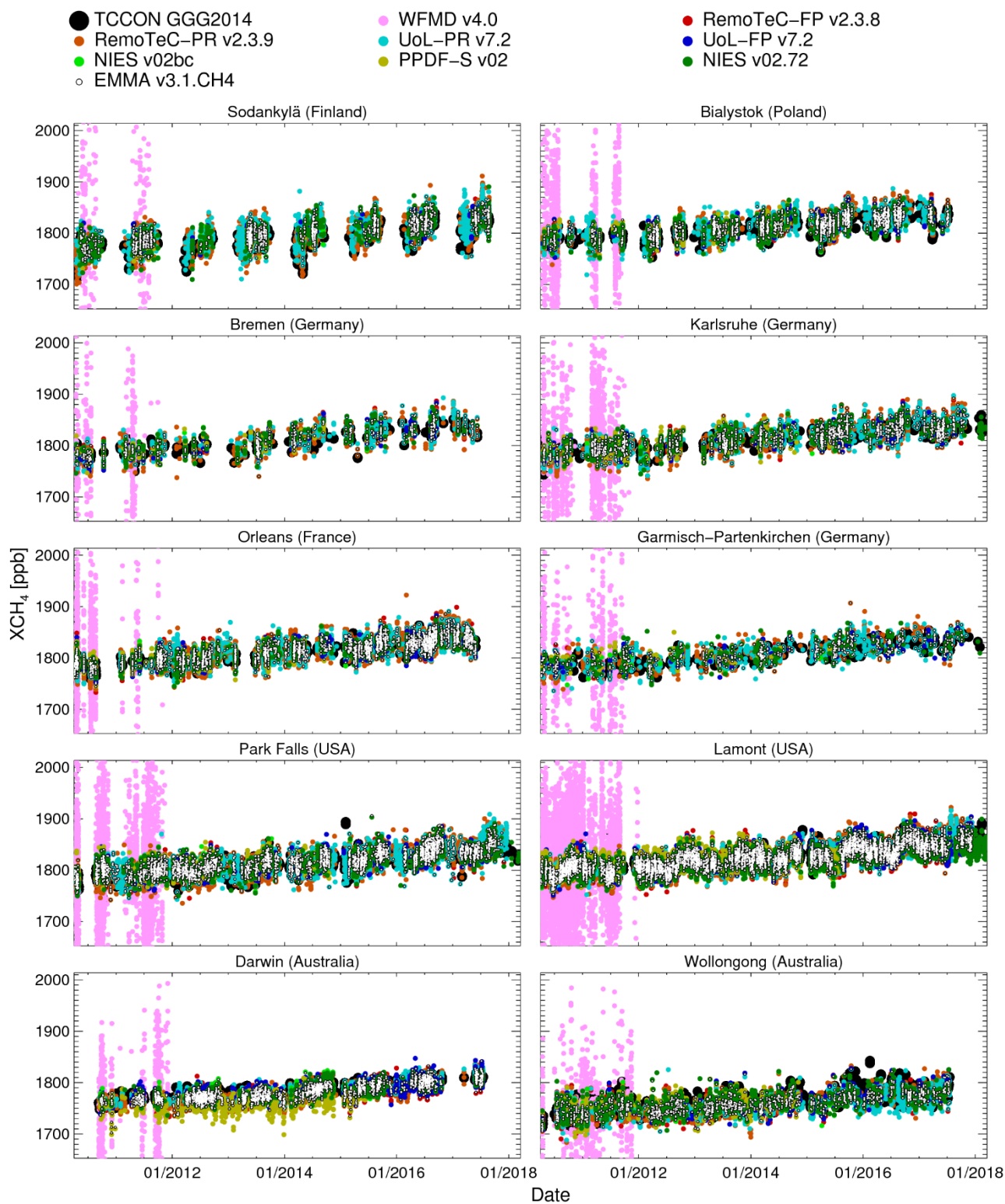


Figure 2: Validation of individual XCH₄ algorithms and EMMA v3.1 CH₄ with TCCON GGG2014.



Input and auxiliary data

1.1 Satellite instrument

At present, several different XCO₂ and XCH₄ retrieval algorithms exist for SCIAMACHY and GOSAT which are under active development in order to meet the demanding user requirements, making them useful for surface flux inversions. Specifically, we here make use of BESD v02.01.02 (*Reuter et al., 2016*), RemoTeC v2.3.8 (*Detmers et al., 2017a*), ACOS v7.3.10a (*O'Dell et al., 2012*), UoL-FP v7.2 (*Boesch and Anand, 2017*), and NIES v02 (*Yoshida et al., 2013*) without and with (v02bc) bias correction, and PPDF-S v02 (*Bril et al., 2012*) for XCO₂ and WFMD v4.0 (*Schneising et al., 2016*), RemoTeC-FP v2.3.8 (*Detmers et al., 2017a*), RemoTeC-PR v2.3.9 (*Detmers et al., 2017b*), UoL-FP v7.2 (*Boesch and Anand, 2017*), UoL-PR v7.2 (*Boesch and Anand, 2017*), and NIES v02 (*Yoshida et al., 2011*) without and with (v02bc) bias correction, and PPDF-S v02 (*Bril et al., 2012*) for XCH₄.

The basic principle of all these algorithms is the same: (i) A satellite instrument measures backscattered solar radiation in near-infrared O₂ and CO₂ or CH₄ absorption bands. (ii) A radiative transfer plus instrument model (forward model) is utilized to simulate the satellite measurement for a set of known parameters (parameter vector) and unknown parameters (state vector). (iii) An inversion method tries to find that state vector which results in best agreement of simulated and measured radiances. (iv) The retrieved state vector is assumed to represent the true (or most likely) atmospheric state.

However, when going into more detail, the algorithms have distinct conceptual differences: the algorithms are optimized for different instruments (SCIAMACHY and GOSAT). They are based on different absorption bands, use different inversion methods (optimal estimation, Tikhonov-Phillips, least squares), and are based on different physical assumptions on the radiative transfer in scattering atmospheres. So-called full physics algorithms explicitly account for (multiple) scattering at molecules, aerosols, and/or clouds by having state vector elements such as cloud water path, cloud top height, and aerosol optical thickness. The light path proxy method assumes that photon path lengths are modified similarly in the CO₂ and O₂ or CH₄ absorption bands, and that scattering related effects cancel out when dividing the retrieved CO₂ and O₂ or CH₄ columns when building XCO₂ or XCH₄. Additionally, the algorithms use different pre- and post-processing filters (e.g., cloud detection from O₂-A band or from a cloud and aerosol imager).

The main properties of the used retrieval algorithms are summarized in **Table 2** and **Table 3**. This list does not claim to be exhaustive and there are other aspects which can also easily result in differences of some ppm (e.g., spectroscopy). Discussions of the specific strengths and weaknesses and many more points, where the individual algorithms differ, can be found in the cited literature.

1.2 Other

In order to account for different column averaging kernels, all retrieval results are adjusted to a common a priori, namely the simple empirical CO₂ model SECM of *Reuter et al. (2012)* or the model based CH₄ climatology adjusted for the annual growth SC4C.



Scaling the reported uncertainties and validation is done with TCCON (total carbon column observing network, *Wunch et al., 2011*) GGG2014 as reference data set.



Algorithms

1.3 Ensemble spread

Due to entirely different samplings (different satellites, different filtering strategies, etc.), any algorithm inter-comparison considering the majority of individual soundings (level 2) can only be based on aggregated data (level 3), in our case monthly averages on a $10^\circ \times 10^\circ$ grid.

Before gridding, we apply the individual averaging kernels to adjust all retrieval results to a common a priori, namely the simple empirical CO_2 model SECM of *Reuter et al. (2012)* or the model based CH_4 climatology adjusted for the annual growth SC4C. We do this as proposed in the textbook of *Rodgers (2000)* and applied to XCO₂ by, for example, *Reuter et al. (2011)*. SECM and SC4C reproduce large-scale features such as the year-to-year increase, the north/south gradient, and the seasonal cycle. However, SECM and SC4C are only empirically extrapolating from past modeled CO_2 and CH_4 fields. New or changing phenomena cannot be within SECM or SC4C, and it should also be mentioned that the adjustments are mostly minor, especially for CO_2 with typically a few tenths of a ppm.

For consistency, we remove the overall global bias of each retrieval with SECM or SC4C as reference. In order to get statistically robust results, we only use those grid boxes with more than five soundings and for which the standard error of the mean is estimated to be less than 1ppm and 12ppb for XCO₂ and XCH₄, respectively. This takes the individual retrieval precisions into account so that the minimum number of soundings needed to build the average of a grid box can vary from retrieval to retrieval and grid box to grid box. Additionally, only grid boxes with a maximum number of overlapping algorithms (see **Figure 3**) are considered for the global bias adjustment. Beforehand, the reported retrieval precision is scaled to match (on average) the precision given in **Table 4** and **Table 5** obtained from a unified validation with TCCON data (**Figure 1** and **Figure 2**). **Figure 4** shows the influence of the global bias correction.

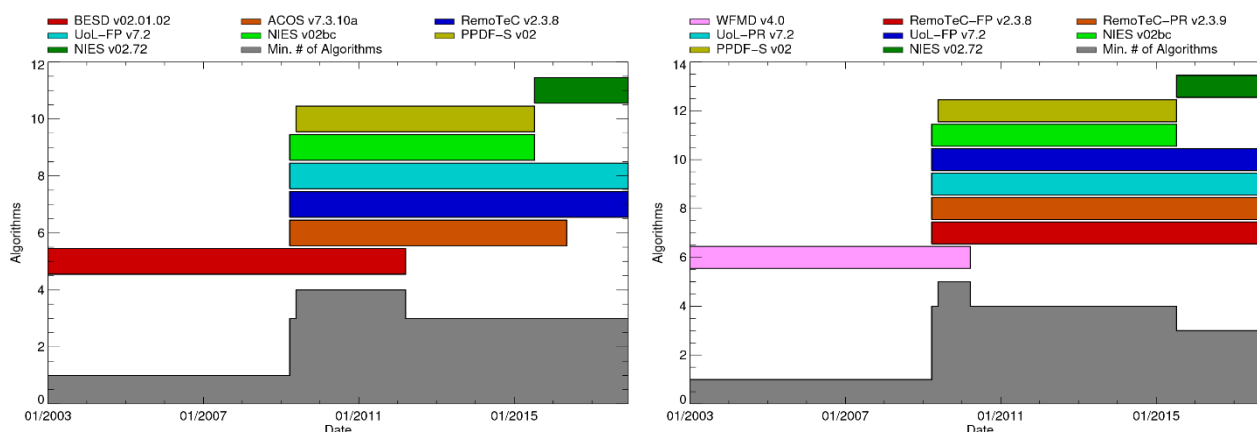


Figure 3: EMMA v3.1 input data availability (colored bars) and minimum number of used algorithms (gray) for median calculation for CO_2 (left) and CH_4 (right).

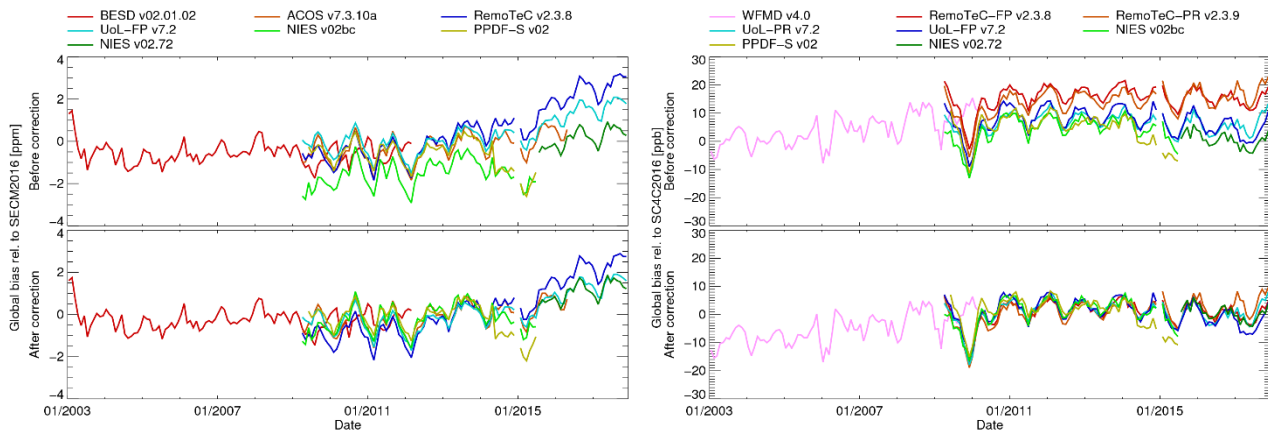


Figure 4: Global monthly average bias for XCO₂ (left) and XCH₄ (right) in common grid boxes relative to SECM (XCO₂) and SC4C (XCH₄) before (top) and after (bottom) global bias correction.

Figure 5 and **Figure 6** show at the example of September 2009 or 2010 the calculated monthly XCO₂ or XCH₄ averages, respectively. First of all, one can see many large scale similarities such as the north/south gradient. However, one can also find more or less obvious outliers in the order of a percent for several algorithms. Often the observed systematic deviations (of level 3 data) are larger than expected from instrumental noise, i.e., they are dominated by specific algorithm effects. As level 3 grid boxes are always calculated from several individual level 2 soundings (ideally) sampled all over the grid box, we expect that sampling and representation errors are lower than the observed deviations. Therefore, these errors are not discussed further in this context.

Due to independent algorithm developments, different physical approaches and assumptions, different pre- and post-processing filters, and due to the different instruments, we expect relatively independent bias patterns. This is supported by **Figure 5** and **Figure 6**, which show (uncorrelated) obvious outliers in various regions, i.e., it seems unlikely that all algorithms produce the same bias within one grid box. This implies that similar averages within one grid box can give us more confidence in the individual retrievals within this grid box. On the other way around, large inter-algorithm spreads indicate regions with more difficult and uncertain retrieval conditions. Therefore, we interpret the ensemble spread, i.e., the standard deviation, as uncertainty due to regional retrieval biases. An example is given in **Figure 7** showing larger inter-algorithm spreads for XCO₂ and XCH₄ in the tropics and in East Asia (always remote from TCCON sites). This pattern is temporally more or less stable, i.e., similar also in other months.

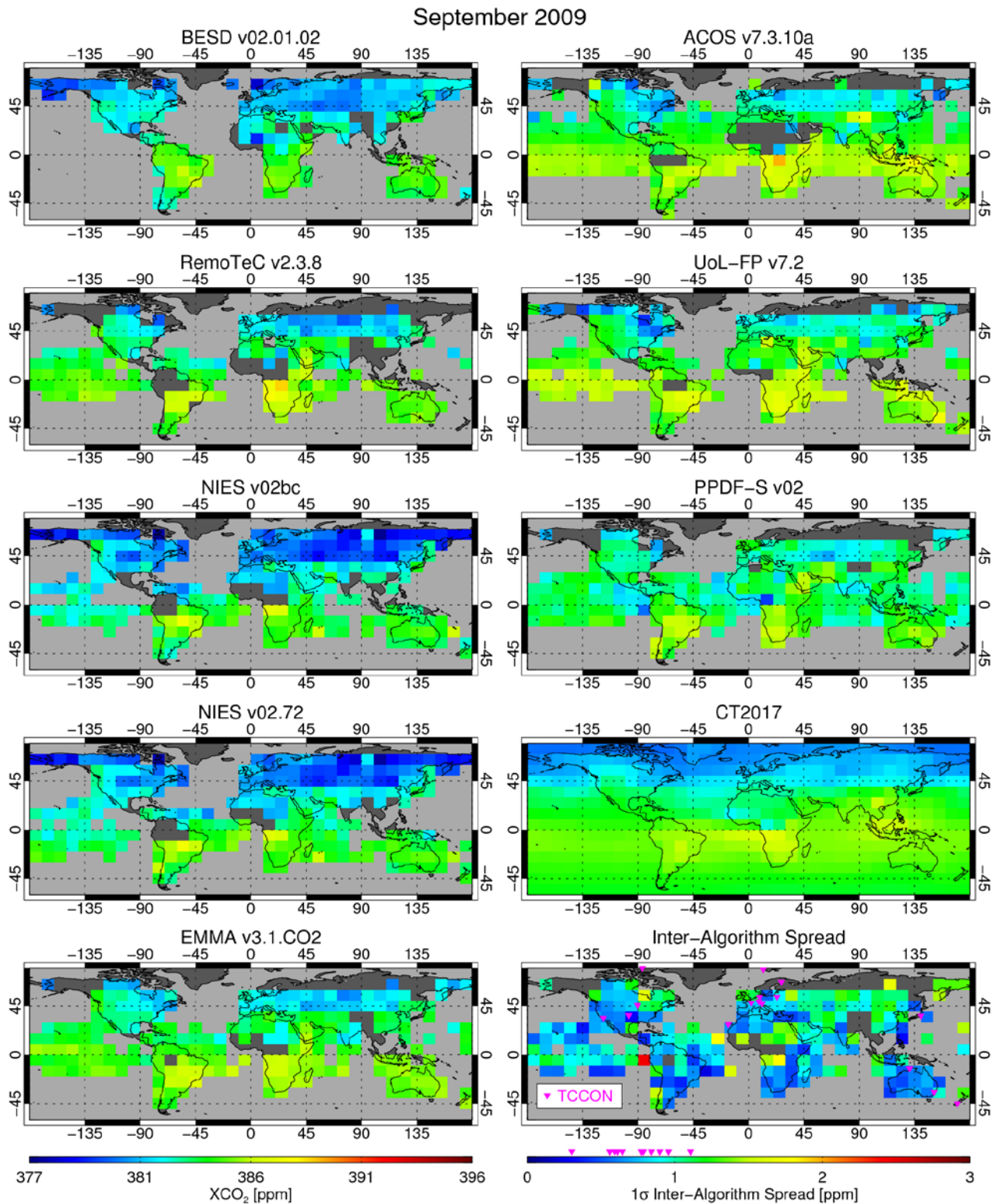


Figure 5: Monthly gridded XCO₂ averages and inter-algorithm spread at the example of September 2009 for EMMA v3.1 CO₂.



September 2010

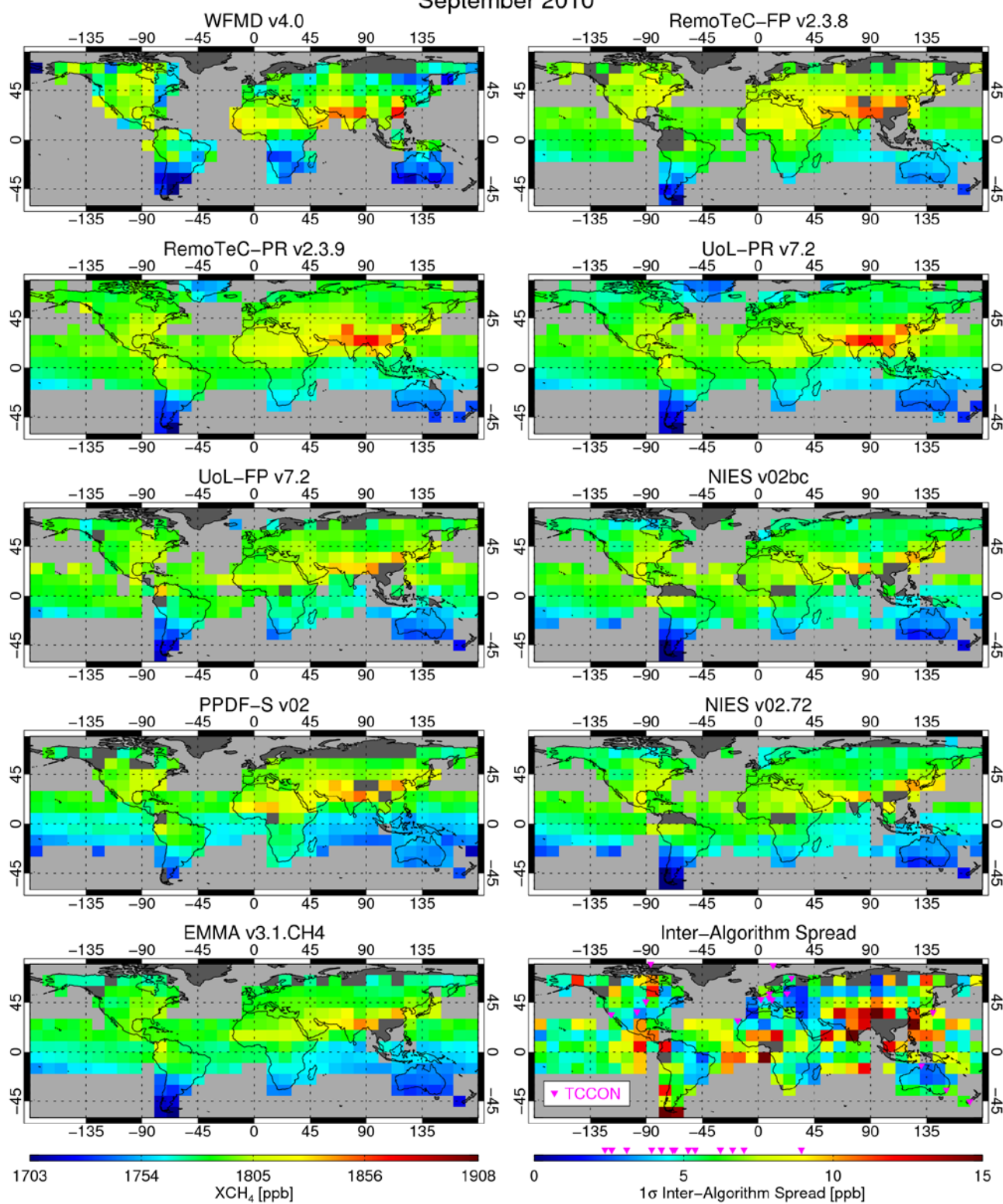




Figure 6: Monthly gridded XCH4 averages and inter-algorithm spread at the example of September 2010 for EMMA v3.1 CH4.

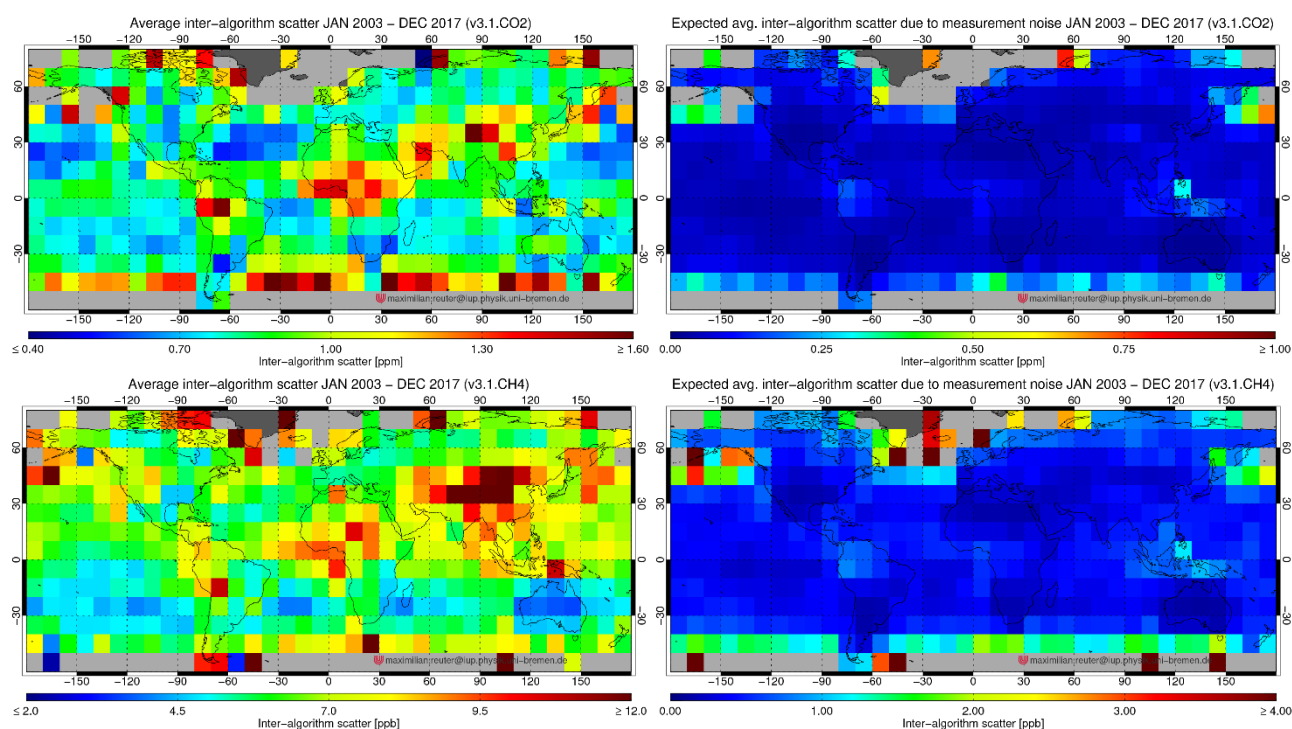


Figure 7: Average inter-algorithm spread (01/2003 – 12/2017) (**left**) and expected average inter-algorithm spread due to measurement noise (**right**) for EMMA v3.1 CO₂ (**top**) and EMMA v3.1 CH₄ (**bottom**).

1.4 Ensemble median

As described in the previous section, XCO₂ or XCH₄ averages (one for each algorithm) are calculated within each grid box. However, now, we are aiming to use the ensemble not only to assess regional and temporal uncertainties but also to create a data set which is potentially less influenced by regional or temporal biases. This could be achieved, for example, by building the average, a weighted average, or the median in each grid box.

In this context, the median has some advantages: outliers are assumed to be seldom and there is a high chance that a grid box includes no or only one outlying algorithm. Therefore, cancellation of errors cannot be expected by calculating the average. The median is much less sensitive to such individual outliers. Additionally, the median calculates no new quantity from the individuals of an ensemble, it is rather a procedure to select one specific ensemble member.

This allows us to trace back from level 3 averages to individual level 2 soundings. Essentially, there are five possible scenarios for median calculation within one grid box: (i) All algorithms perform well and scatter slightly around the true XCO₂ or XCH₄ value. In this case the median will help to reduce scatter. (ii) The minority of algorithms produce outliers so that the median is influenced only



marginally. (iii) The majority of algorithms produce outliers in different directions. Here, it is still likely that the median falls on a well performing algorithm in the “middle”. (iv) The majority of algorithms produce outliers in the same direction. This is the only case where the median is a bad choice, because it would select an outlier and ignore a well performing algorithm. As discussed in the previous section, we assume that the algorithms within one grid box are often realistic with uncorrelated occasional outliers, which makes this case unlikely to happen often. (v) If all algorithms are outlying, the median is not better or worse than selecting any other ensemble member.

We calculate the median only in grid boxes where reliable average XCO₂ or XCH₄ values can be computed for at least as many algorithms as specified in **Figure 3** (gray area). In case of an even number of values, we define the median as that value being closer to the mean. We then trace back to the individual level 2 data, which were used to calculate that average being the median. Together, with all information needed for inverse modeling (geo-location, time, averaging kernels, etc.), these soundings are stored in the EMMA database.

Some algorithms may provide considerably larger amounts of level 2 data (e.g., WFMD, weighting function modified DOAS) than other algorithms. In order to prevent over-weighting these algorithms, we limit the maximum number of data points (per grid box). Therefore, we calculate the standard error of the mean of each successfully determined average. The idea behind this is that the lower the standard error of the mean, the larger the potential constraint on an inverse model becomes. If the standard error of the mean of the selected algorithm in a grid box is lower than $1/\sqrt{2}$ times the 25% percentile of all algorithms, the data points are randomly thinned accordingly. In this way, the number of data points can still be rather different but the potential constraint on an inverse model becomes similar.



Output data

The EMMA database consists of individual level 2 soundings retrieved by algorithms which can change from grid box to grid box and month to month. Therefore, it can be used in the same manner as any other XCO₂ or XCH₄ satellite retrieval. **Figure 8** shows the relative data weight of each algorithm (defined as $\sum 1/\sigma_i^2$ normalized to one) within the EMMA database per month. The EMMA database includes all information needed for inverse modeling (geo-location, time, XCO₂ or XCH₄, averaging kernels, etc.). Additionally, it includes the inter-algorithm spread which informs about potential regional uncertainties.

At the example of September 2009 or 2010, **Figure 9** shows the EMMA v3.1 XCO₂ or XCH₄ values as well as the corresponding selected median algorithm.

Note that the format of the main output data, which are the Level 2 data products, is described in the separate Product User Guide and Specification (PUGS) document.

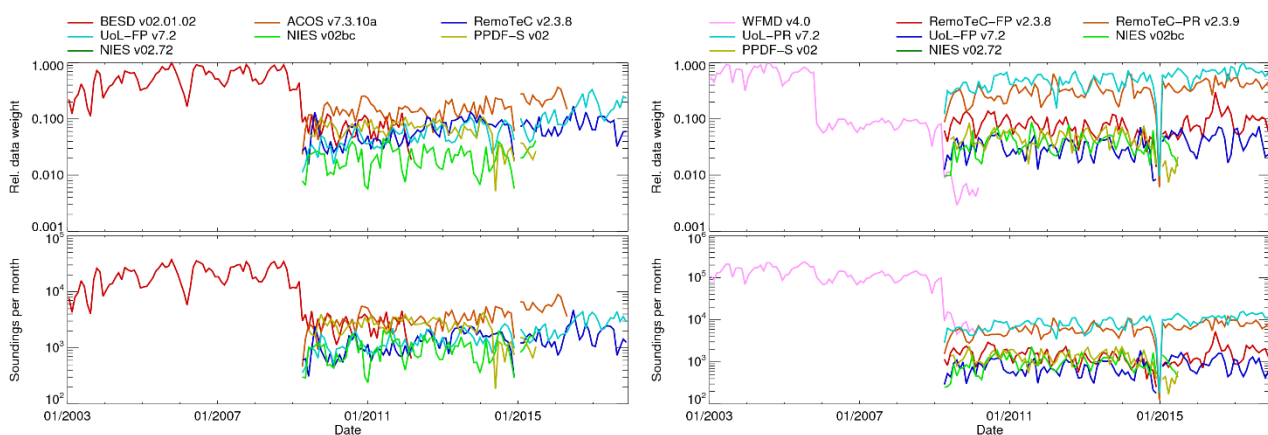


Figure 8: EMMA v3.1 normalized relative data weight proportional to $\sum 1/\sigma_i^2$ (top) and number of soundings (bottom) per algorithm and month for CO₂ (left) and CH₄ (right).

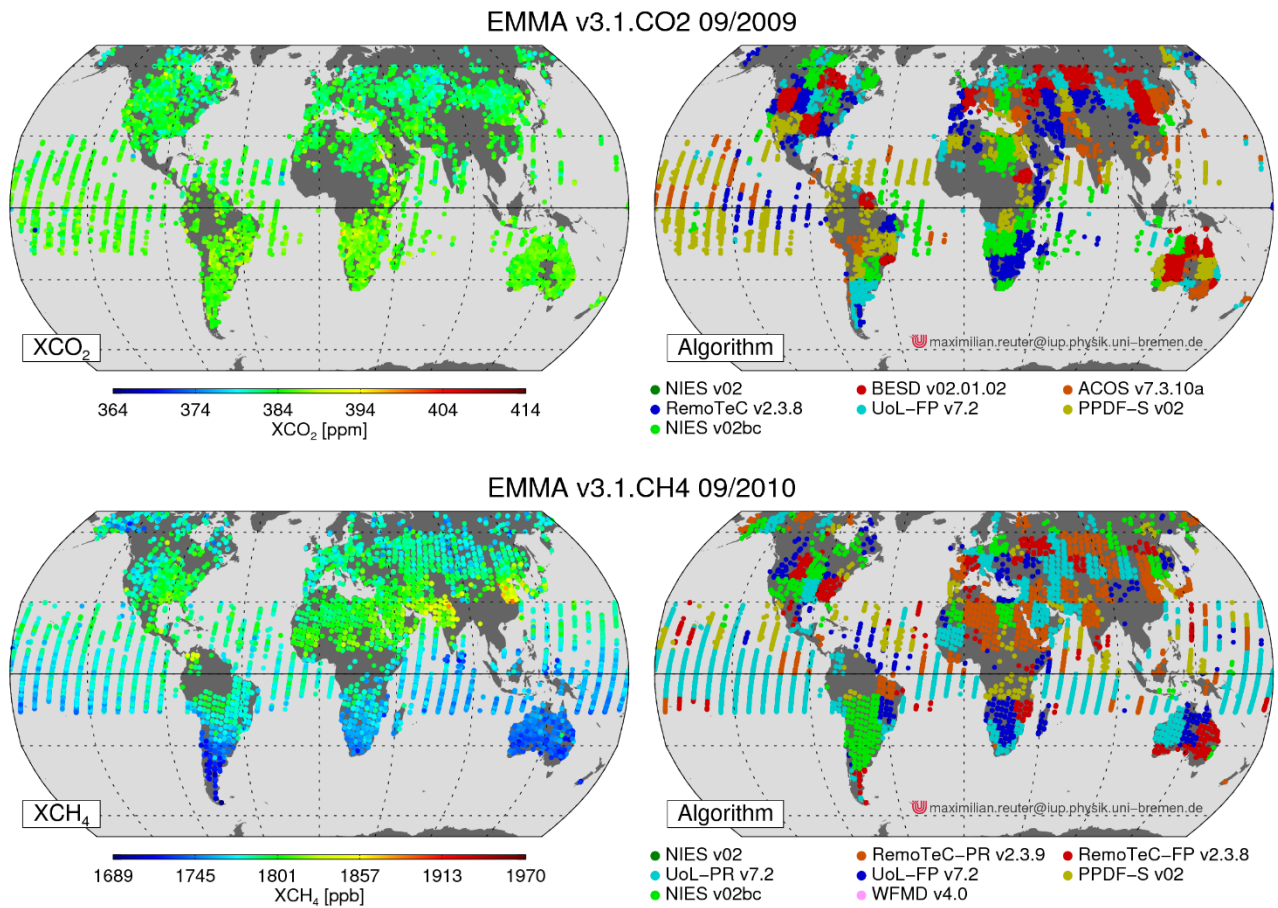


Figure 9: EMMA L2 XCO₂ and XCH₄ (**left**) and corresponding selected algorithm (**right**) for EMMA v3.1 CO₂ at the example of September 2009 (**top**) and EMMA v3.1 CH₄ at the example of September 2010 (**bottom**).



References

- Araujo and New, 2007:** Araujo, M. B. and New, M.: Ensemble forecasting of species distributions, *Trends Ecol. Evol.*, 22, 42–47, doi:10.1016/j.tree.2006.09.010, 2007
- Boesch and Anand, 2017:** H. Boesch and J. Anand, Algorithm Theoretical Basis Document (ATBD) – ANNEX A for products CO₂_GOS_OCFP, CH₄_GOS_OCFP & CH₄_GOS_OCP, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO₂ and CH₄) data products (project C3S_312a_Lot6), Version 1 (21/08/2017), 2017
- Bovensmann et al., 1999:** Bovensmann, H., Burrows, J. P., Buchwitz, M., Frerick, J., Noel, S., Rozanov, V. V., Chance, K. V., and Goede, A.: SCIAMACHY – Mission Objectives and Measurement Modes, *J. Atmos. Sci.*, 56, 127–150, 1999
- Bril et al., 2012:** Bril, A.; Oshchepkov, S.; Yokota, T. Application of a probability density function-based atmospheric light-scattering correction to carbon dioxide retrievals from GOSAT over-sea observations. *Remote Sensing of the Environment* 2012, 117, 301–306
- Burrows et al., 1995:** Burrows, J. P., Hölzle, E., Goede, A. P. H., Visser, H., and Fricke, W.: SCIAMACHY – Scanning Imaging Absorption Spectrometer for Atmospheric Chartography, *Acta Astronaut.*, 35, 445–451, 1995
- Chevallier et al., 2007:** Chevallier, F., Bréon, F.-M., and Rayner, P. J.: Contribution of the Orbiting Carbon Observatory to the estimation of CO₂ sources and sinks: Theoretical study in a variational data assimilation framework, *J. Geophys. Res.*, 112, D09307, doi:10.1029/2006JD007375, 2007
- Detmers, 2017a:** R. Detmers, Algorithm Theoretical Basis Document (ATBD) – ANNEX B for products CO₂_GOS_SRFP & CH₄_GOS_SRFP, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO₂ and CH₄) data products (project C3S_312a_Lot6), Version 1 (21/08/2017), 2017
- Detmers, 2017b:** R. Detmers, Algorithm Theoretical Basis Document (ATBD) – ANNEX C for product CH₄_GOS_SRPR, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases (CO₂ and CH₄) data products (project C3S_312a_Lot6), Version 1 (21/08/2017), 2017
- Hagedorn et al., 2005:** Hagedorn, R., Doblas-Reyes, F., and Palmer, T.: The rationale behind the success of multi-model ensembles in seasonal forecasting – I. Basic concept, *Tellus A*, 57, 219–233, doi:10.1111/j.1600-0870.2005.00103.x, 2005
- Houweling et al., 2014:** Houweling, S., Breon, F.-M., Aben, I., Rötodenbeck, C., Gloor, M., Heimann, M., and Ciais, P.: Inverse modeling of CO₂ sources and sinks using satellite data: a synthetic inter-comparison of measurement techniques and their performance as a function of space and time, *Atmos. Chem. Phys.*, 4, 523–538, doi:10.5194/acp-4-523-2004, 2004
- Karion et al., 2010:** Karion, A., Sweeney, C., Tans, P., and Newberger, T.: AirCore: An Innovative Atmospheric Sampling System, *J. Atmos. Ocean. Tech.*, 27, 1839–1853, doi:10.1175/2010JTECHA1448.1, 2010



- Miller et al., 2007:** Miller, C. E., Crisp, D., DeCola, P. L., Olsen, S. C., Randerson, J. T., Michalak, A. M., Alkhaled, A., Rayner, P., Jacob, D. J., Suntharalingam, P., Jones, D. B. A., Denning, A. S., Nicholls, M. E., Doney, S. C., Pawson, S., Bösch, H., Connor, B. J., Fung, I. Y., O'Brien, D., Salawitch, R. J., Sander, S. P., Sen, B., Tans, P., Toon, G. C., Wennberg, P. O., Wofsy, S. C., Yung, Y. L., and Law, R. M.: Precision requirements for space-based XCO₂ data, *J. Geophys. Res.*, 112, D10314, doi:10.1029/2006JD007659, 2007
- O'Dell et al., 2012:** O'Dell, C. W., Connor, B., Bösch, H., O'Brien, D., Frankenberg, C., Castano, R., Christi, M., Eldering, D., Fisher, B., Gunson, M., McDuffie, J., Miller, C. E., Natraj, V., Oyafo, F., Polonsky, I., Smyth, M., Taylor, T., Toon, G. C., Wennberg, P. O., and Wunch, D.: The ACOS CO₂ retrieval algorithm – Part 1: Description and validation against synthetic observations, *Atmos. Meas. Tech.*, 5, 99–121, doi:10.5194/amt-5-99-2012, 2012
- Rayner and O'Brien, 2001:** Rayner, P. J. and O'Brien, D. M.: The utility of remotely sensed CO₂ concentration data in surface inversions, *Geophys. Res. Lett.*, 28, 175–178, 2001
- Reuter et al., 2011:** M. Reuter, H. Bovensmann, M. Buchwitz, J. P. Burrows, B. J. Connor, N. M. Deutscher, D. W. T. Griffith, J. Heymann, G. Keppel-Aleks, J. Messerschmidt, J. Notholt, C. Petri, J. Robinson, O. Schneising, V. Sherlock, V. Velasco, T. Warneke, P. O. Wennberg, D. Wunch: Retrieval of atmospheric CO₂ with enhanced accuracy and precision from SCIAMACHY: Validation with FTS measurements and comparison with model results. *Journal of Geophysical Research - Atmospheres*, 116, D04301, doi: 10.1029/2010JD015047, 2011
- Reuter et al., 2012:** M. Reuter, M. Buchwitz, O. Schneising, F. Hase, J. Heymann, S. Guerlet, A. J. Cogan, H. Bovensmann, J. P. Burrows: A simple empirical model estimating atmospheric CO₂ background concentrations. *Atmospheric Measurement Techniques*, doi:10.5194/amt-5-1349-2012, 5, 1349-1357, 2012
- Reuter et al., 2016:** M. Reuter, H. Bovensmann, M. Buchwitz, J. P. Burrows, J. Heymann, O. Schneising, Algorithm Theoretical Basis Document Version 5 (ATBDv5) - The Bremen Optimal Estimation DOAS (BESD) algorithm for the retrieval of XCO₂, ESA Climate Change Initiative (CCI) for the Essential Climate Variable (ECV) Greenhouse Gases (GHG), Version 5, 2016
- Reuter et al., 2017:** M. Reuter, H. Bösch, H. Bovensmann, A. Bril, M. Buchwitz, A. Butz, J. P. Burrows, C. W. O'Dell, S. Guerlet, O. Hasekamp, J. Heymann, N. Kikuchi, S. Oshchepkov, R. Parker, S. Pfeifer, O. Schneising, T. Yokota, and Y. Yoshida: A joint effort to deliver satellite retrieved atmospheric CO₂ concentrations for surface flux inversions: the ensemble median algorithm EMMA. *Atmospheric Chemistry and Physics*, doi:10.5194/acp-13-1771-2013, 13, 1771-1780, 2013
- Rötter et al., 2011:** Rötter, R. P., Carter, T. R., Olesen, J. E., and Porter, J. R.: Cropclimate models need an overhaul, *Nat. Clim. Change*, 1, 175–177, 2011
- Rodgers 2000:** Rodgers, C. D.: *Inverse Methods for Atmospheric Sounding: Theory and Practice*, World Scientific Publishing, Singapore, 2000
- Schneising et al., 2016:** GHG-CCI group at IUP Bremen, Algorithm Theoretical Basis Document (ATBD) - SCIAMACHY WFM-DOAS (WFMD) XCO₂ and XCH₄ for the Essential Climate Variable (ECV)



Greenhouse Gases (GHG), ESA Climate Change Initiative (CCI) for the Essential Climate Variable (ECV) Greenhouse Gases (GHG), Version 5, 2016

Tebaldi, C. and Knutti, 2007: Tebaldi, C. and Knutti, R.: The use of the multi-model ensemble in probabilistic climate projections, *Philos. Trans. R. Soc. A*, 365, 2053–2075, doi:10.1098/rsta.2007.2076, 2007

Vautard et al., 2009: Vautard, R., Schaap, M., Bergstrom, R., Bessagnet, B., Brandt, J., Builtjes, P. J. H., Christensen, J. H., Cuvelier, C., Foltescu, V., Graff, A., Kerschbaumer, A., Krol, M., Roberts, P., Rouil, L., Stern, R., Tarrason, L., Thunis, P., Vignati, E., and Wind, P.: Skill and uncertainty of a regional air quality model ensemble, *Atmos. Environ.*, 43, 4822–4832, doi:10.1016/j.atmosenv.2008.09.083, 2009

Wunch et al., 2011: Wunch, D., Toon, G. C., Blavier, J.-F. L., Washenfelder, R. A., Notholt, J., Connor, B. J., Griffith, D. W. T., Sherlock, V., and Wennberg, P. O.: The Total Carbon Column Observing Network (TCCON), *Phil. Trans. R. Soc. A*, 369, 2087–2112, doi:10.1098/rsta.2010.0240, 2011

Yokota et al., 2004: Yokota, T., Oguma, H., Morino, I., and Inoue, G.: A nadir looking SWIR sensor to monitor CO₂ column density for Japanese GOSAT project, *Proceedings of the twenty-fourth international symposium on space technology and science*, Miyazaki: Japan Society for Aeronautical and Space Sciences and ISTS, 887–889, 2004

Yoshida et al., 2011: Yoshida, Y., Ota, Y., Eguchi, N., Kikuchi, N., Nobuta, K., Tran, H., Morino, I., and Yokota, T.: Retrieval algorithm for CO₂ and CH₄ column abundances from short-wavelength infrared spectral observations by the Greenhouse gases observing satellite, *Atmos. Meas. Tech.*, 4, 717–734, doi:10.5194/amt-4-717-2011, 2011

Copernicus Climate Change Service

ECMWF - Shinfield Park, Reading RG2 9AX, UK

Contact: info@copernicus-climate.eu

climate.copernicus.eu

copernicus.eu

ecmwf.int