



# Global satellite observations of column-averaged carbon dioxide and methane: The GHG-CCI XCO<sub>2</sub> and XCH<sub>4</sub> CRDP3 data set

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## ► To cite this version:

M. Buchwitz, M. Reuter, O. Schneising, W. Hewson, R.G. Detmers, et al.. Global satellite observations of column-averaged carbon dioxide and methane: The GHG-CCI XCO<sub>2</sub> and XCH<sub>4</sub> CRDP3 data set. Remote Sensing of Environment, 2017, 203, pp.276-295. 10.1016/J.RSE.2016.12.027 . hal-02951858

**HAL Id: hal-02951858**

**<https://hal.science/hal-02951858>**

Submitted on 24 Jun 2021

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**Global satellite observations of column-averaged carbon dioxide and methane:  
The GHG-CCI XCO<sub>2</sub> and XCH<sub>4</sub> CRDP3 data set**

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**Abstract**

Carbon dioxide (CO<sub>2</sub>) and methane (CH<sub>4</sub>) are the two most important greenhouse gases emitted by mankind. Better knowledge of the surface sources and sinks of these Essential Climate Variables (ECVs) and related carbon uptake and release processes is needed for important climate change related applications such as improved climate modelling and prediction. Some satellites provide near-surface-sensitive atmospheric CO<sub>2</sub> and CH<sub>4</sub> observations that can be used to obtain information on CO<sub>2</sub> and CH<sub>4</sub> surface fluxes. The goal of the GHG-CCI project of the European Space Agency's (ESA) Climate Change Initiative (CCI) is to use satellite data to generate atmospheric CO<sub>2</sub> and CH<sub>4</sub> data products meeting demanding GCOS (Global Climate Observing System) greenhouse gas (GHG) ECV requirements. To achieve this, retrieval algorithms are regularly being improved followed by annual data reprocessing and analysis cycles to generate better products in terms of extended time series and continuously improved data quality. Here we present an overview about the latest GHG-CCI data set called Climate Research Data Package No. 3 (CRDP3) focusing on the GHG-CCI core data products, which are column-averaged dry-air mole fractions of CO<sub>2</sub> and CH<sub>4</sub>, i.e., XCO<sub>2</sub> and XCH<sub>4</sub>, as retrieved from SCIAMACHY/ENVISAT and TANSO/GOSAT satellite radiances covering the time period end of 2002 to end of 2014. We present global maps and time series including initial validation results obtained by comparisons with Total Carbon Column Observing Network (TCCON) ground-based observations. We show that the GCOS requirements for systematic error (< 1 ppm for XCO<sub>2</sub>, < 10 ppb for XCH<sub>4</sub>) and long-term stability (< 0.2 ppm/year for XCO<sub>2</sub>, < 2 ppb/year for XCH<sub>4</sub>) are met for nearly all products (an exception is SCIAMACHY methane especially since 2010). For XCO<sub>2</sub> we present comparisons with global models using the output of two CO<sub>2</sub> assimilation systems (MACC version 14r2 and CarbonTracker version CT2013B). We show that overall there is reasonable consistency and agreement between all data sets (within ~1-2 ppm) but we also found significant differences depending on region and time period.

## 1. Introduction

Carbon dioxide (CO<sub>2</sub>) is the most important human-emitted greenhouse gas responsible for global warming (IPCC, 2013). Despite its importance, our knowledge of the CO<sub>2</sub> sources and sinks has significant gaps and does not meet all needs for attribution, mitigation and the accurate prediction of future climate change (e.g., Stephens et al., 2007; Canadell et al., 2010; IPCC, 2013; Ciais et al., 2014). Despite efforts to reduce CO<sub>2</sub> emissions, atmospheric CO<sub>2</sub> continues to increase with currently approximately 2 ppm/year (e.g., Fig. 1 (satellite-derived column-averaged CO<sub>2</sub>) and Le Quéré et al., 2015, based on Dlugokencky and Tans, 2015, NOAA/ESRL (near) surface CO<sub>2</sub> concentrations). The situation is similar for methane (CH<sub>4</sub>; e.g., Dlugokencky et al., 2009; IPCC, 2013; Kirschke et al., 2013; Houweling et al., 2014; Alexe et al., 2015).

The goal of the GHG-CCI project (Buchwitz et al., 2015), which is one of several projects of ESA's Climate Change Initiative (CCI, Hollmann et al., 2013), is to generate global satellite-derived atmospheric CO<sub>2</sub> and CH<sub>4</sub> data sets with as high as possible new information content on regional CO<sub>2</sub> and CH<sub>4</sub> sources and sinks, i.e., surface fluxes, to be extracted, for example, via inverse modeling (e.g., Reuter et al., 2014a; Alexe et al., 2015). GHG-CCI generates data sets of the Essential Climate Variable (ECV) Greenhouse Gases (GHG) as required by the GCOS (Global Climate Observing System) defined as follows (GCOS, 2011): "Product Number A.8.1: Retrievals of greenhouse gases, such as CO<sub>2</sub> and CH<sub>4</sub>, of sufficient quality to estimate regional sources and sinks".

Currently multi-year radiance measurements from two satellite instruments are used in GHG-CCI to retrieve information on atmospheric CO<sub>2</sub> and CH<sub>4</sub> with high near-surface-sensitivity: SCIAMACHY on ENVISAT (2002 - April 2012) (Burrows et al., 1995; Bovensmann et al., 1999) and TANSO-FTS on-board GOSAT (launched in 2009) (Kuze et al., 2009, 2014). Both instruments perform (or have performed) nadir observations in the near-infrared/short-wave-infrared (NIR/SWIR) spectral region covering the relevant absorption bands of CO<sub>2</sub>, CH<sub>4</sub> and molecular oxygen (O<sub>2</sub>). The latter is used to obtain the “dry-air column” needed to compute GHG column-averaged dry-air mole fractions, i.e., XCO<sub>2</sub> (in ppm) and XCH<sub>4</sub> (in ppb) from the retrieved GHG vertical columns (e.g., Buchwitz et al., 2005) and/or to obtain information on atmospheric scatterers, e.g., on aerosols and thin cirrus clouds. These two instruments are the two main sensors used within GHG-CCI but in the future other sensors with similar radiance observations may be added, e.g., NASA’s successfully launched OCO-2 mission for XCO<sub>2</sub> (Crisp et al., 2004; Bösch et al., 2011; Zhang et al., 2016) and ESA’s Sentinel-5-Precursor mission for XCH<sub>4</sub> (Veefkind et al., 2012; Butz et al., 2012).

During recent years significant progress has been made towards achieving the demanding satellite XCO<sub>2</sub> and XCH<sub>4</sub> requirements. Prior to the GHG-CCI project initial XCO<sub>2</sub> retrievals were available from SCIAMACHY (e.g., Buchwitz et al., 2005, 2007; Schneising et al., 2008, 2009) but only first preliminary GOSAT retrievals. Progress has been made in terms of improved data quality, time coverage and interpretation of satellite XCO<sub>2</sub> data products (using GHG-CCI and other products generated in Japan (e.g., Yoshida et al., 2013, Oshchepkov et al., 2011, 2013) and in the USA (e.g., O’Dell et al., 2012; Crisp et al., 2012)) to enhance our knowledge on the various sources and sinks of these gases (e.g., Basu et al., 2013; Maksyutov et al., 2013; Saeki et al., 2013; Chevallier et al., 2014; Takagi et al., 2014; Reuter et al., 2014a, 2014b; Houweling et al., 2015; Alexe et al., 2015).

For example, focusing on hemispheric data and on carbon-climate feedbacks, Schneising et al., 2014a, used SCIAMACHY XCO<sub>2</sub> retrievals to study aspects related to the terrestrial carbon sink by looking at co-variations of XCO<sub>2</sub> growth rates and seasonal cycle amplitudes with near-surface temperature. They found XCO<sub>2</sub> growth rate changes of 1.25 $\pm$ 0.32 ppm/year/K (approximately 2.7 $\pm$ 0.7

GtC/year/K; indicating less carbon uptake in warmer years consistent with a positive carbon-climate feedback) for the Northern Hemisphere in good agreement with CarbonTracker. The CO<sub>2</sub> seasonal cycle, which is driven primarily by terrestrial CO<sub>2</sub> uptake and release processes, has also been studied in several other publications (e.g., Reuter et al., 2013; Buchwitz et al., 2015; Lindqvist et al., 2015). Guerlet et al., 2013, analyzed GOSAT XCO<sub>2</sub> retrievals focusing on the Northern Hemisphere. They identified reduced carbon uptake in the summer of 2010 and found that this is most likely due to the heat wave in Eurasia driving biospheric fluxes and fire emissions. Using a joint inversion of GOSAT and surface data, they estimated an integrated biospheric and fire emission anomaly in April–September 2010 of  $0.89 \pm 0.20$  PgC over Eurasia. Basu et al., 2014, studied seasonal variations of CO<sub>2</sub> fluxes during 2009–2011 over Tropical Asia using GOSAT, CONTRAIL and IASI data. They found an enhanced source for 2010 and concluded that this is likely due to the biosphere response to above-average temperatures in 2010 and unlikely due to biomass burning emissions. Parazoo et al., 2013, used GOSAT XCO<sub>2</sub> and solar induced chlorophyll fluorescence (SIF) retrievals to better understand the carbon balance of southern Amazonia. Ross et al., 2013, used GOSAT data to obtain information on wildfire CH<sub>4</sub>:CO<sub>2</sub> emission ratios. For flux inversions not only the retrieved greenhouse gas values are relevant but also their error statistics, in particular the reported uncertainties. Chevallier and O’Dell, 2013, analyzed this aspect in the context of CO<sub>2</sub> flux inversions using GOSAT XCO<sub>2</sub> retrievals. Detmers et al., 2015, analyzed GOSAT XCO<sub>2</sub> to detect and quantify anomalously large climate-related carbon uptake in Australia during the time period end of 2010 to early 2012. Furthermore, a number of publications focused on improving retrieval algorithms including data processing and comparisons with ground-based observations and global models (e.g. Heymann et al., 2012a, 2012b) or on applying existing algorithms to other sensors (e.g., Heymann et al., 2015). Satellite XCO<sub>2</sub> retrievals are also used, for example by the European Centre for Medium-Range Weather Forecasts (ECMWF), to characterize atmospheric CO<sub>2</sub> at large and synoptic scales and for CO<sub>2</sub> forecasting (Massart et al., 2016). Last but not least and despite the fact that none of the existing satellite missions has been optimized to obtain information on anthropogenic CO<sub>2</sub> emissions (in contrast to other proposed future missions, in particular CarbonSat (Bovensmann et al., 2010; Velazco et al., 2011; Buchwitz et al., 2013)) this important aspect has been addressed in several recent

publications using existing satellite XCO<sub>2</sub> products (Kort et al., 2012; Schneising et al., 2013, Reuter et al., 2014b).

Nevertheless, not all carbon-related problems which have been addressed can be answered with confidence due to potential issues with the satellite retrievals (in particular remaining biases) and/or transport modelling (e.g., Stephens et al., 2007) as needed to interpret the satellite products (e.g., Chevallier et al., 2010; Deng et al., 2014). An example is the recent effort to quantify European biospheric terrestrial CO<sub>2</sub> fluxes. Basu et al., 2013, presented first CO<sub>2</sub> surface flux inverse modeling results from GOSAT XCO<sub>2</sub> retrievals for various regions including Europe. For Europe their results imply that Europe is a much stronger carbon sink than current knowledge suggests. Chevallier et al., 2014a, used an ensemble of inversion methods and GOSAT XCO<sub>2</sub> retrievals to also derive regional (sub-continental) CO<sub>2</sub> surface fluxes. They also found a significantly larger European carbon sink. They conclude that the derived sink is unrealistically large and they argue that this may be due to modelling issues related to long-range transport modelling and/or biases of the satellite retrievals. In particular they argue that errors of the satellite data outside of Europe may adversely influence the European results. To further investigate this European carbon sink issue in detail, Reuter et al., 2014a, used an ensemble of SCIAMACHY and GOSAT XCO<sub>2</sub> data products and an inversion method which is not, or at least significantly less, sensitive to the potential issues discussed in Chevallier et al., 2014a. For example, Reuter et al., 2014a, only used satellite XCO<sub>2</sub> retrievals over Europe to rule out that non-European satellite data adversely influence the results for the European carbon sink and they also only used short-term (days) transport modelling for satellite data interpretation to minimize potential long-range transport errors. Reuter et al., 2014a, also performed several sensitivity tests to investigate the robustness of their results and to establish a reliable error budget. Based on an extensive analysis they conclude: “We show that the satellite-derived European terrestrial carbon sink is indeed much larger (1.02 +/- 0.30 GtC/year in 2010) than previously expected”. The value they derived is larger compared to earlier inversion estimates using in-situ observations of 0.47 +/- 0.50 (“LSCE-39-insitu inversion”) or 0.42 +/- 0.25 (“UoE-insitu”) GtC/year for 2010 (Chevallier et al., 2014a), or 0.40 +/- 0.42 GtC/year for 2001-2004 (Peylin et al., 2013), which is reported in the recent

IPCC report (IPCC, 2013). The disagreement with bottom-up estimates is even larger and significant: Schulze et al., 2009, report  $0.235 \pm 0.05$  GtC/year between 2000 and 2005. These findings of Reuter et al., 2014a, stimulated additional research using satellite and non-satellite CO<sub>2</sub> observations (e.g., Feng et al., 2016, and discussion in Houweling et al., 2015) but consensus has not yet been achieved, e.g., Feng et al., 2016, finally conclude: "...we cannot prove or disprove that European ecosystems are taking up a larger-than-expected amount of CO<sub>2</sub>". Recently, some new research results have been obtained by assimilating new Siberian CO<sub>2</sub> observations in CarbonTracker (Kim et al., 2016). They report a European sink strength of  $0.75 \pm 0.63$  GtC/year for 2008-2009, which temporally overlaps with the range reported by Reuter et al., 2014a, and is significantly larger compared to their reference inversions without these new Siberian observations. On the other hand, based on simultaneous CO<sub>2</sub> and CH<sub>4</sub> flux inversions using GOSAT-retrieved ratios of total column CH<sub>4</sub> and CO<sub>2</sub> for 2009 and 2010, Pandey et al., 2016, obtain European terrestrial CO<sub>2</sub> fluxes close to zero, in contrast to the results discussed above. Apparently, more research is needed to answer this important European carbon sink question with confidence.

For satellite XCH<sub>4</sub> retrievals and the interpretation of these data sets the situation is similar as for XCO<sub>2</sub>. SCIAMACHY data have already been extensively used to improve our knowledge on atmospheric methane and regional methane emissions prior to the start of the GHG-CCI project (e.g., Buchwitz et al., 2005; Frankenberg et al., 2005; Schneising et al., 2009; Bergamaschi et al., 2007, 2009; Bloom et al., 2010). A more recent research focus has been to investigate the unexpected renewed atmospheric methane increase since 2007 using ground-based and/or satellite data (e.g., Rigby et al., 2008; Dlugokencky et al., 2009; Bergamaschi et al., 2009, 2013; Schneising et al., 2011; Frankenberg et al., 2011; Sussmann et al., 2012; Crevoisier et al., 2013; Houweling et al., 2014; Nisbet et al., 2014; Schaefer et al., 2016). Methane emission estimates have been obtained from GOSAT as discussed in a number of recent publications (e.g., Fraser et al., 2013, 2014, Monteil et al., 2013, Cressot et al., 2014, Alexe et al., 2015; Turner et al., 2015, 2016). In these studies often CH<sub>4</sub> retrievals from several satellites have been used (as well as other data, in particular NOAA data), e.g., Monteil et al., 2013, and Alexe et al., 2015, used SCIAMACHY and GOSAT retrievals, Cressot et al., 2014, used

GOSAT, SCIAMACHY and IASI, and Wecht et al., 2014, and Worden et al., 2015, used GOSAT and TES satellite retrievals. Several publications focused on relatively localized methane sources, e.g., in the United States: For example, Schneising et al., 2014, analyzed SCIAMACHY data over major US “fracking” regions and quantified anthropogenic methane emissions and leakage rates and also others used SCIAMACHY data over the US to identify and quantify localized methane emission sources (Kort et al., 2014; Wecht et al., 2014). The SCIAMACHY XCH<sub>4</sub> retrievals have also been used to compare with and to improve chemistry-climate models (Shindell et al., 2014, Hayman et al., 2014).

Despite this quite large number of publications it is clear that still much more has to be learned about the various (and changing) sources and sinks of CO<sub>2</sub> and CH<sub>4</sub>. It is obvious that the more accurate and precise the observations are and the longer and denser the observational time series is, the larger their information content. Within the GHG-CCI project a continuous algorithm improvement, re-processing and data product analysis cycle is carried out every year with the goal to deliver each year an improved data set of satellite-derived atmospheric CO<sub>2</sub> and CH<sub>4</sub> information. The latest data set is called CRDP3. This data set is presented in the following (Sect. 2) including an initial quality assessment by comparison with ground-based observations (Sect. 3) and model comparisons (Sects. 4 and 5) focusing on CO<sub>2</sub>. A summary and conclusions are given in Sect. 6.

## **2. Overview data set CRDP3**

The GHG-CCI latest data set called Climate Research Data Package No. 3 (CRDP3) consists of several satellite-derived atmospheric CO<sub>2</sub> and CH<sub>4</sub> data products. These data products are classified as (i) GHG-CCI project core products, generated with so-called ECV Core Algorithms (ECAs), and (ii) additional products, generated with so-called Additional Constraints Algorithms (ACAs). The ECA products are XCO<sub>2</sub> and XCH<sub>4</sub> (see Tabs. 1 and 2) retrieved from satellite nadir mode radiance spectra in the near-infrared / shortwave-infrared (NIR/SWIR) spectral region using appropriate retrieval algorithms. These retrieval algorithms are all based on modelling the observed radiance spectra using a radiative transfer model and corresponding parameters (e.g., vertical profiles of atmospheric CO<sub>2</sub>,

CH<sub>4</sub>, temperature, aerosols, etc.) coupled to an inversion method to iteratively optimize selected parameters until the modeled radiance matches the observed radiance spectrum. All retrieval algorithms are based on Optimal Estimation / Bayesian Inference theory (see Rodgers, 2000, for the general theory and Reuter et al., 2010, for a typical example) with the exception of the WFMD algorithms (see Tabs. 1 and 2), which are based on a least-squares fitting combined with a very fast look-up-table scheme (e.g., Buchwitz et al., 2000; Schneising et al., 2011). The algorithms are also using post-processing steps including bias correction and quality filtering and/or assigning a quality flag to each single retrieval (ground pixel) (see information on retrieval Algorithm Theoretical Baseline Documents (ATBDs) given below).

**Table 1:** Overview GHG-CCI individual ECV Core Algorithms (ECAs) as used for XCO<sub>2</sub> retrieval and the generation of the corresponding data product. See main text for a description of baseline and alternative products.

<b>GHG-CCI ECV Core Algorithms (ECAs) for XCO<sub>2</sub> retrieval</b>			
<b>Algorithm ID (Version)</b>	<b>Sensor</b>	<b>Algorithm Institute</b>	<b>Comment (Algorithm reference)</b>
CO2_SCI_BESD (v02.01.01)	SCIAMACHY/ ENVISAT	BESD IUP, Univ. Bremen, Germany	SCIAMACHY XCO <sub>2</sub> baseline product Coverage: global (land), 1.2003-3.2012 (Reuter et al., 2011)
CO2_SCI_WFMD (v3.9)	—	WFM-DOAS IUP, Univ. Bremen, Germany	SCIAMACHY XCO <sub>2</sub> alternative product Coverage: global (land), 10.2002-4.2012 (Schneising et al., 2011)
CO2_GOS_OCFP (v6.0)	TANSO/GOSAT	UoL-FP University of Leicester (UoL), UK	GOSAT XCO <sub>2</sub> baseline product Coverage: global, 4.2009-12.2014 (Cogan et al., 2012)
CO2_GOS_SRFP (v2.3.7)	—	RemoTeC SRON (Utrecht, Netherlands) & KIT (Karlsruhe, Germany)	GOSAT XCO <sub>2</sub> alternative product Coverage: global, 6.2009-12.2014 (Butz et al., 2011)

225 **Table 2:** As Tab. 1 but for the GHG-CCI individual XCH<sub>4</sub> retrieval algorithms and corresponding data  
 226 products.

<b>GHG-CCI ECV Core Algorithms (ECAs) for XCH<sub>4</sub> retrieval</b>			
<b>Algorithm ID (Version)</b>	<b>Sensor</b>	<b>Algorithm Institute</b>	<b>Comment (Algorithm reference)</b>
CH4_SCI_WFMD (v3.9)	SCIAMACHY/ ENVISAT	WFM-DOAS IUP, Univ. Bremen, Germany	SCIAMACHY XCH <sub>4</sub> proxy product (baseline not yet decided) Coverage: global, 10.2002-12.2011 (Schneising et al., 2011)
CH4_SCI_IMAP (v7.1)	--	IMAP SRON (Utrecht, Netherlands) & JPL (Padadena, CA, USA)	SCIAMACHY XCH <sub>4</sub> proxy product (baseline not yet decided) Coverage: global (land), 1.2003-4.2012 (Frankenberg et al., 2011)
CH4_GOS_OCPR (v6.0)	TANSO/GOSAT	UoL-PR University of Leicester (UoL), UK	GOSAT XCH <sub>4</sub> proxy baseline product Coverage: global, 4.2009-12.2014 (Parker et al., 2011)
CH4_GOS_SRPR (v2.3.7)	--	RemoTeC SRON (Utrecht, Netherlands) & KIT (Karlsruhe, Germany)	GOSAT XCH <sub>4</sub> proxy alternative product Coverage: global, 6.2009-12.2014 (Butz et al., 2010)
CH4_GOS_SRFP (v2.3.7)	--	RemoTeC SRON (Utrecht, Netherlands) & KIT (Karlsruhe, Germany)	GOSAT XCH <sub>4</sub> full physics baseline product Coverage: global, 6.2009-12.2014 (Butz et al., 2011)
CH4_GOS_OCFP (v1.0)	--	UoL-PR University of Leicester (UoL), UK	GOSAT XCH <sub>4</sub> full physics alternative product Coverage: global, 4.2009-12.2014 (Parker et al., 2011)

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The exploited NIR/SWIR spectral regions contain relevant CO<sub>2</sub>, CH<sub>4</sub> and (depending on algorithm/product) molecular oxygen (O<sub>2</sub>) absorption lines. O<sub>2</sub> is used to get information on the light path and on the dry-air column needed to convert the GHG vertical columns into mole fractions (number density mixing ratio). For sufficiently cloud-free day-side observations these spectra are typically dominated by surface-reflected solar radiation and are therefore sensitive to near-surface greenhouse gas concentration variations.

Currently, the corresponding GHG-CCI ECA products are derived from SCIAMACHY/ENVISAT and TANSO/GOSAT. In this publication we focus on the GHG-CCI CRDP3 ECA products. An overview on the additional GHG-CCI ACA products is given in Buchwitz et al., 2015, and details are given on the GHG-CCI website (<http://www.esa-ghg-cci.org/>), in particular in the corresponding ACA product tables as given on the GHG-CCI main data products website ([http://www.esa-ghg-cci.org/sites/default/files/documents/public/documents/GHG-CCI\\_DATA.html](http://www.esa-ghg-cci.org/sites/default/files/documents/public/documents/GHG-CCI_DATA.html)). In short, ACA products are not (or typically not) sensitive to near-surface GHG variations but to variations in upper atmospheric layers, i.e., layers above the planetary boundary layer. They therefore provide complementary additional information (compared to ECAs) on atmospheric CO<sub>2</sub> and CH<sub>4</sub>. ACA products are mid/upper tropospheric CO<sub>2</sub> and CH<sub>4</sub> mixing ratios from IASI (Crevoisier et al., 2009a, 2009b, 2013), upper tropospheric / stratospheric vertical CH<sub>4</sub> profiles from MIPAS (Laeng et al., 2015), stratospheric CH<sub>4</sub> and CO<sub>2</sub> profiles from SCIAMACHY solar occultation observations (Noël et al., 2012, 2016) and stratospheric CO<sub>2</sub> profiles from ACE-FTS (Foucher et al., 2009).

An overview about the GHG-CCI ECAs and corresponding data products is given in Tab. 1 for XCO<sub>2</sub> and in Tab. 2 for XCH<sub>4</sub>. As can be seen, there are two algorithms for each data product. For example, there are two algorithms for XCO<sub>2</sub> from SCIAMACHY and two algorithms for XCO<sub>2</sub> from GOSAT, resulting in four XCO<sub>2</sub> products generated independently with different algorithms. We encourage users of our data products to take advantage of this ensemble of products which can even be extended using additional (i.e., non-GHG-CCI) products generated elsewhere, most notably in Japan (NIES products (Yoshida et al., 2013; Oshchepkov et al., 2011, 2013) and in the USA (NASA ACOS product

(O'Dell et al., 2012; Crisp et al., 2012)). The main reason for this recommendation is that even small (and typically difficult to characterize) systematic errors in the XCO<sub>2</sub> products can lead to quite large errors when using XCO<sub>2</sub> to get information on CO<sub>2</sub> surface fluxes (emission or uptake). This is because the CO<sub>2</sub> background concentration is quite high and even large sources and sinks typically results in only small XCO<sub>2</sub> variations (see, e.g., Reuter et al., 2014a). Using an ensemble of products generated with independent algorithms enables one to determine the robustness of the source/sink findings with respect to algorithmic choices which have to be made when implementing a retrieval algorithm and also permits one to assign more realistic error bars to quantitative source/sink results (see, for example, Reuter et al., 2014a, using an ensemble of XCO<sub>2</sub> data products to obtain information on the strength of the European carbon sink).

However, we acknowledge that this is a major effort which cannot be undertaken by all users, e.g., due to time, financial or other constraints. For these users we aim at giving recommendations on which product to use if they can or want to use only one (or a few) products. We do this by identifying so-called baseline (or recommended) products (see also Buchwitz et al., 2015, and Dils et al., 2014, for our initial “Round Robin” attempt to identify “best” algorithms and corresponding data products). As can be seen from Tabs. 1 and 2, we have identified baseline algorithms/products for all products except for SCIAMACHY XCH<sub>4</sub> (as both products still suffer from degraded quality as discussed below). Note that a baseline product is not necessarily significantly better than the corresponding alternative product because, as one may expect, different algorithms have different strengths and weaknesses. Often we found that data products differ (e.g., at the different individual validation sites) but it is not clear which one is better (e.g., if the overall agreement with the validation network is on average equivalently good). Therefore, for products where this is the case, the baseline product is for some products simply the product which has been agreed upon between the different data providing institutions. Note that the definition of “better” also depends on the application. For example, for SCIAMACHY XCO<sub>2</sub>, the BESD product has been declared as baseline product and the WFMD product as alternative product because BESD has typically lower systematic errors / biases, and better precision, i.e., less random errors (as confirmed by the results shown in Sect. 3.1) but much less data

(approx. 50% as also shown in Sect. 3.1) compared to the WFMD product. For some applications with relevant requirements on spatio-temporal coverage, the WFMD product may therefore be the better suited or even the only choice provided the biases are small enough for the target application. Within the GHG-CCI project quality assessment is an ongoing effort with one of the goals to confirm or change the classification of algorithms/products as “baseline” or “alternative”, depending on future algorithm improvements and corresponding future data quality.

Note that two additional XCO<sub>2</sub> and XCH<sub>4</sub> products are available from the GHG-CCI website not listed in Tabs. 1 and 2. These are the Ensemble Median Algorithm (EMMA) XCO<sub>2</sub> (Reuter et al., 2013) and XCH<sub>4</sub> products. These products are also Level 2 products (i.e., non-gridded individual ground pixel swath products) as the other products listed in Tabs. 1 and 2 but they have been generated by merging individual products from SCIAMACHY and GOSAT. They are not further discussed here (for details see Reuter et al., 2013, and Buchwitz et al., 2016).

As can be seen from Tab. 2, the number of XCH<sub>4</sub> algorithms/products is even larger than for XCO<sub>2</sub>. The reason is that there are two types of XCH<sub>4</sub> algorithms for the GOSAT products, the so-called (light path) “proxy” (PR) algorithms and the “full-physics” (FP) algorithms (see Schepers et al., 2012, Buchwitz et al., 2015, Parker et al., 2015, and references given therein for details). In short, XCH<sub>4</sub> PR algorithms convert retrieved CH<sub>4</sub> columns into XCH<sub>4</sub> by using dry-air columns obtained from simultaneously retrieved CO<sub>2</sub> column in combination with modelled CO<sub>2</sub> column to correct for CO<sub>2</sub> column variations (the PR algorithm require that atmospheric CH<sub>4</sub> columns typically vary more than CO<sub>2</sub> columns (in relative, i.e., percentage, terms)). The advantage of the PR method is that systematic column retrieval errors (e.g., light path errors due to unaccounted scattering by aerosols and clouds but also some instrument errors) cancel to some extent when the ratio of the retrieved CH<sub>4</sub> and CO<sub>2</sub> columns is computed. The disadvantage is that this method needs sufficiently accurate CO<sub>2</sub> model simulations to correct for CO<sub>2</sub> variations. The FP method, which does not have this disadvantage, aims at considering aerosol and cirrus effects explicitly by considering (as good as possible) the “full physics” of the atmospheric radiative transfer. This means that FP methods aim at solving a much

more challenging radiative transfer and inversion problem and, therefore, they do not have to rely on accurate CO<sub>2</sub> modelling. This shows that both methods have different strengths and weaknesses. As a consequence the resulting data products have different characteristics (typically PR products contain much more data points compared to FP products, see Sect. 3.2). Because these two type of methane algorithms/products are significantly different they are classified separately as baseline or alternative as shown in Tab. 2.

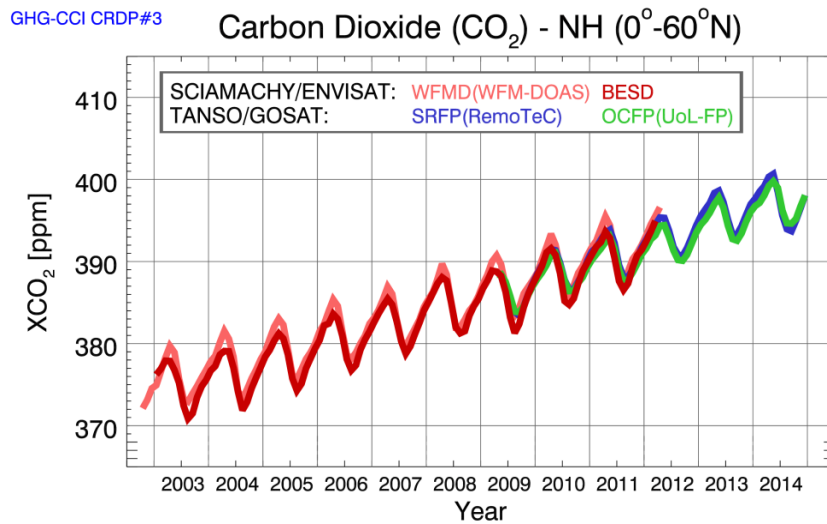
Despite the fact that all algorithms are based on similar principles (namely on optimizing radiative transfer model and other parameters until a “good” match between the measured and modelled radiances has been obtained), they differ in many details. It is out of the scope of this manuscript to explain each algorithm in detail. Instead we refer to the documentation as given on the GHG-CCI website, in particular to the Algorithm Theoretical Baseline Documents (ATBDs) (see links given in the product tables of the GHG-CCI main data products website ([http://www.esa-ghg-cci.org/sites/default/files/documents/public/documents/GHG-CCI\\_DATA.html](http://www.esa-ghg-cci.org/sites/default/files/documents/public/documents/GHG-CCI_DATA.html))).

Figure 1 shows time series of northern hemispheric XCO<sub>2</sub> as obtained from all four GHG-CCI XCO<sub>2</sub> retrieval algorithms (see Tab. 1). As can be seen, all XCO<sub>2</sub> products clearly show an approximately 2 ppm/year CO<sub>2</sub> increase (due to anthropogenic CO<sub>2</sub> emissions) and the atmospheric CO<sub>2</sub> seasonal cycle (primarily due to regular uptake and release of CO<sub>2</sub> by the terrestrial biosphere). The SCIAMACHY products cover (essentially) the entire ENVISAT time period from end of 2002 (WFMD product) or beginning of 2003 (BESD product) to April 2012. The GOSAT CRDP3 products cover the time period mid 2009 to end of 2014. As can be seen, the agreement between the different time series is within about 1-2 ppm. Note that perfect agreement is not to be expected, e.g., due to differences in spatio-temporal sampling and vertical sensitivity (see the following sections for quantitative assessments). To obtain quantitative estimates of the characteristics of the various data products in terms of random and systematic errors and long-term stability one has to compare the individual products with appropriate high-quality reference data (see Sect. 3) and one also has to compare spatial pattern (Sect. 4). In Sect. 3 we present comparisons of the satellite products with ground-based observations at selected

locations and in Sect. 4 we present comparison with global models. Note that we also aim at model independent quantitative comparisons of the global satellite data via the Ensemble Median Algorithm EMMA (Reuter et al., 2013). For the latest EMMA assessment results (not shown here) see Buchwitz et al., 2016.

Figure 2 shows time series of northern hemispheric  $XCH_4$ . As can be seen, the agreement among the various products is less good (in relative terms) compared to  $XCO_2$  in particular for the two SCIAMACHY  $XCH_4$  products which also deviate significantly from the GOSAT  $XCH_4$  products in particular for 2010 and later years. This is potentially due to SCIAMACHY detector issues whose impact on the data quality is still large but hopefully can be (further) mitigated in future versions of the SCIAMACHY products. The seasonality of the GOSAT  $XCH_4$  OCFP product, which is a new product from Univ. Leicester, deviates somewhat from the other products. Also this aspect needs further investigation.

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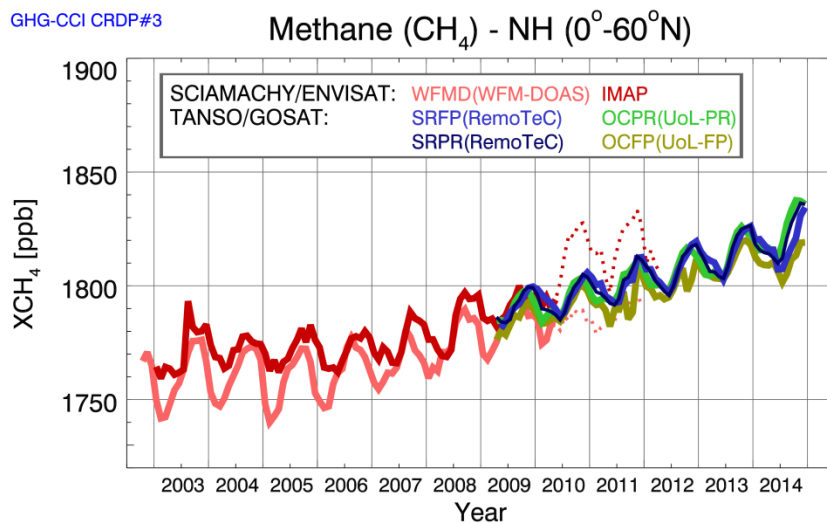


357

358 **Figure 1:** Timeseries of northern hemispheric XCO<sub>2</sub> of the four GHG-CCI CRDP3 XCO<sub>2</sub> data  
359 products (CO2\_SCI\_WFMD (light red), CO2\_SCI\_BESD (red), CO2\_GOS\_SRFP (blue) and  
360 CO2\_GOS\_OCFP (green)) obtained by averaging all satellite retrievals north of the equator up to  
361 60°N for each month.

362

363



364

365 **Figure 2:** Timeseries of northern hemispheric XCH<sub>4</sub> of the six GHG-CCI CRDP3 XCH<sub>4</sub> data products  
366 (see inset) obtained by averaging all satellite retrievals north of the equator up to 60°N for each month.  
367 Note that the SCIAMACHY products after approx. mid 2010 (see dotted lines) suffer from currently  
368 still unresolved issues probably related to detector degradation.

In the following section a comparison of these XCO<sub>2</sub> and XCH<sub>4</sub> products with ground-based reference observations is presented which has been carried out to obtain initial quantitative information on the data quality. Note that a more detailed comparison with ground-based data is presented in Dils et al., 2016.

### 3. Comparisons with ground-based observations

The ground-based Total Carbon Column Observing Network (TCCON) has been designed for validation of satellite XCO<sub>2</sub> and/or XCH<sub>4</sub> retrievals (Wunch et al., 2011a, 2011b) and TCCON data have been used extensively also in the past for comparison of GHG-CCI data products (e.g., Dils et al., 2014, Buchwitz et al., 2015). TCCON is a network of ground-based Fourier Transform Spectrometers recording direct solar spectra in the near-infrared spectral region. From these spectra, accurate and precise column-averaged abundance of CO<sub>2</sub>, CH<sub>4</sub> and other atmospheric data products are retrieved. The TCCON XCO<sub>2</sub> and XCH<sub>4</sub> data products version GGG2014 as used for this study (Wunch et al., 2015) have been downloaded from the TCCON data archive (<http://tccon.ornl.gov>).

Within GHG-CCI we use several somewhat different methods for satellite – TCCON comparison (see Buchwitz et al., 2016) including methods developed and applied independently by each data provider to his/her product. Two methods are applied to all CRDP3 XCO<sub>2</sub> and XCH<sub>4</sub> products, the method developed by the GHG-CCI validation team (Dils et al. 2016) and a somewhat simplified approach developed and used primarily for Quality Control / Quality Assurance (QC/QA) purposes. Overall it has been found that all validation methods result in similar conclusions concerning the overall data quality of the CRDP3 ECA products, which demonstrates the robustness of the findings (Buchwitz et al., 2016). In the following we present the QC/QA approach and its results.

For QC/QA of the CRDP3 ECA products we have used version GGG2014 (Wunch et al., 2015) XCO<sub>2</sub> and XCH<sub>4</sub> TCCON data products from six TCCON sites, two in the USA, two in Europe and two in

Australia (see Tab. 3). For each ECA product and each of the selected TCCON sites we have performed detailed comparisons of individual (but also averaged) satellite soundings (ground pixels) using a co-location criterion of 2 hours temporally and  $4^{\circ} \times 4^{\circ}$  latitude/longitude spatially. To minimize the impact of different *a priori* information used for the retrievals, common CO<sub>2</sub> and CH<sub>4</sub> profiles have been used for comparison using TCCON *a priori* profiles as common profiles for the comparisons (see also Dils et al., 2014, using the same approach).

**Table 3:** TCCON sites and corresponding data coverage as used for comparison with the satellite XCO<sub>2</sub> and XCH<sub>4</sub> data products. The “Time coverage” corresponds to the time coverage of the data products at the time of data access (6-Oct-2015, except Bremen and Bialystok: 20-Nov-2015).

TCCON validation sites					
Location (TCCON data product reference)	Site ID	Latitude [deg]	Longitude [deg]	Altitude [km]	Time coverage MM/YYYY-MM/YYYY
ParkFalls, USA (Wennberg et al., 2014a)	PAR	45.945	-90.273	0.442	06/2004 - 12/2014
Lamont, USA (Wennberg et al., 2014b)	LAM	36.604	-97.486	0.320	07/2008 - 12/2014
Bremen, Germany (Notholt et al., 2014)	BRE	53.104	8.850	0.027	01/2007 - 10/2014
Bialystok, Poland (Deutscher et al., 2014)	BIA	53.231	23.025	0.183	03/2009 - 10/2014
Darwin, Australia (Griffith et al., 2014a)	DAR	-12.425	130.891	0.030	08/2005 - 09/2014
Wollongong, Australia (Griffith et al., 2014b)	WOL	-34.406	150.879	0.030	06/2008 - 09/2014

When interpreting satellite-TCCON differences one also has to consider the uncertainty of the TCCON data products. TCCON uncertainties are reported in the TCCON data product files for each individual observation and these uncertainties have been used, e.g., to avoid using TCCON data with large reported errors. However, what is also needed, in particular to compute systematic satellite-TCCON differences across several sites (see, e.g., summary values for regional and seasonal biases in Tabs. 4 and 5) is an estimate of the TCCON site-to-site bias and/or an estimate of the TCCON uncertainty after averaging many TCCON retrievals. Site-to-site biases for TCCON products are reported in Wunch et al., 2010. As shown in Wunch et al., 2010, the uncertainty of the TCCON data products is typically 0.4 ppm for XCO<sub>2</sub> (1-sigma) and 4 ppb (1-sigma) for XCH<sub>4</sub> (see also the discussion of this and corresponding implications for interpreting satellite - TCCON comparisons as reported in Dils et al., 2014, and Buchwitz et al., 2015). Due to these uncertainties / potential errors of the TCCON data (but also for other reasons, e.g., non-perfect spatio-temporal co-location) the estimated systematic and random errors of the satellite retrievals as reported here have to be interpreted as upper limit estimates (because we assume here that the TCCON site-to-site bias is zero), i.e., the satellite data product errors are likely smaller than reported here, at least at the TCCON sites. On the other hand the TCCON network is quite sparse and does not cover all geophysical conditions. For example, for the XCO<sub>2</sub> products it has been identified that differences between satellite products located far away from TCCON sites may differ by somewhat larger amounts than the TCCON validation suggests (e.g., Reuter et al., 2013). Because of these potential overestimation (neglect of TCCON site-to-site bias) / underestimation (TCCON does not capture all situation) issues we interpret the differences to TCCON reported here as a reasonable estimate of the real error (which can be compared with the user requirements) without taking the uncertainty of the TCCON retrievals explicitly into account, i.e., we assume that underestimation and overestimation effects cancels to a large extent (at least on average).

As shown in the following two sub-sections, we compare the achieved performance with the required performance as specified by GCOS (GCOS, 2011) and with the typically more demanding and more detailed requirements as specified in the GHG-CCI User Requirements Document (URD, Chevallier et

al., 2014b). Note that GCOS is not explicitly specifying requirements for XCO<sub>2</sub> and XCH<sub>4</sub> but for „Tropospheric CO<sub>2</sub> column“ and „Tropospheric CH<sub>4</sub> column“ in mole fraction (mixing ratio) units (e.g., ppm for CO<sub>2</sub>). In this manuscript we interpret the GCOS requirements as listed in GCOS, 2011, as requirements for XCO<sub>2</sub> and XCH<sub>4</sub>.

**Table 4:** Comparison results for product CO2\_SCI\_BESD with TCCON XCO<sub>2</sub> at six TCCON sites. In the top part of the table results are listed per TCCON site. Reported in column “Bias” are the regional and seasonal biases (see main text for details), the “Scatter”, which is the standard deviation of satellite-TCCON difference (based on the individual satellite soundings, i.e., ground pixel) and “RepUncert” (reported uncertainty), which is the mean value of the reported uncertainty as given in the satellite product files for each single sounding. “UncRat” is the uncertainty ratio, which is the ratio of RepUnc and Scatter. Values close to unity indicate that the reported uncertainty is (on average) reliable. “Trend” characterises the long-term stability as obtained by fitting a straight line to the satellite minus TCCON differences covering the entire time series. The listed trend error is the 3-sigma uncertainty of the slope of the fitted line. Nobs are the number of individual satellite soundings compared to TCCON. In the bottom part of the table summary values are listed for each parameter (the sum or the mean and/or the standard deviation). See main text for details.

Site ID	Bias [ppm]		Scatter [ppm]	RepUnc [ppm] (UncRat [-])	Trend (Stability) [ppm/year]	Nobs [-]
	Regional	Seasonal				
PAR	-0.2	0.8	2.0	2.1 (1.0)	0.14 +/- 0.04	2931
LAM	-0.3	0.7	1.7	1.9 (1.1)	-0.01 +/- 0.05	12003
BRE	-0.3	0.8	1.8	2.5 (1.4)	-0.13 +/- 0.13	1036
BIA	-0.2	1.0	2.0	1.9 (1.0)	0.03 +/- 0.17	1124
DAR	-0.5	0.9	1.8	1.7 (0.9)	-0.02 +/- 0.04	7323
WOL	0.5	0.6	2.2	2.1 (0.9)	-0.07 +/- 0.11	2389
<b>Summary:</b>						
Sum						26806
Mean	-0.2	0.8	1.9	2.0 (1.1)	-0.01 +/- 0.09	
StdDev	0.4					

455

456 **Table 5:** As Tab. 4 but for product CH4\_SCI\_WFMD.

Site ID	Bias [ppb]		Scatter [ppb]	RepUnc [ppb] (UncRat [-])	Trend (Stability) [ppb/year]	Nobs [-]
	Regional	Seasonal				
PAR	5.0	19.6	78.2	67.3 (0.9)	0.77 +/- 0.84	11079
LAM	4.5	10.5	75.1	84.1 (1.1)	0.23 +/- 2.00	18725
BRE	2.9	18.4	91.8	85.8 (0.9)	-1.86 +/- 4.80	1512
BIA	6.2	18.9	88.8	84.2 (0.9)	6.88 +/- 7.62	2230
DAR	-18.1	17.2	67.9	82.7 (1.2)	-1.87 +/- 1.38	10580
WOL	-16.2	16.4	88.0	82.0 (0.9)	7.73 +/- 5.34	2832
<b>Summary:</b>						
Sum						46958
Mean	-2.6	16.8	81.6	81.0 (1.0)	1.98 +/- 3.66	
StdDev	11.3					

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459 **3.1 XCO<sub>2</sub> comparisons with TCCON**

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461 Figure 3 shows as an example a comparison of the CO2\_SCI\_BESD product with TCCON XCO<sub>2</sub>

462 retrievals at Lamont, Oklahoma, USA. As can be seen, several figures of merit are listed in Fig. 3.

463 They have been defined and computed for quantitative characterization of systematic and random

464 errors of the satellite products and to determine if there are linear trends in the satellite-TCCON

465 differences, i.e., to assess the long-term stability of the satellite products. We also aim at validating the

466 reported uncertainty, which is given in the GHG-CCI data products for each single retrieval (i.e., for

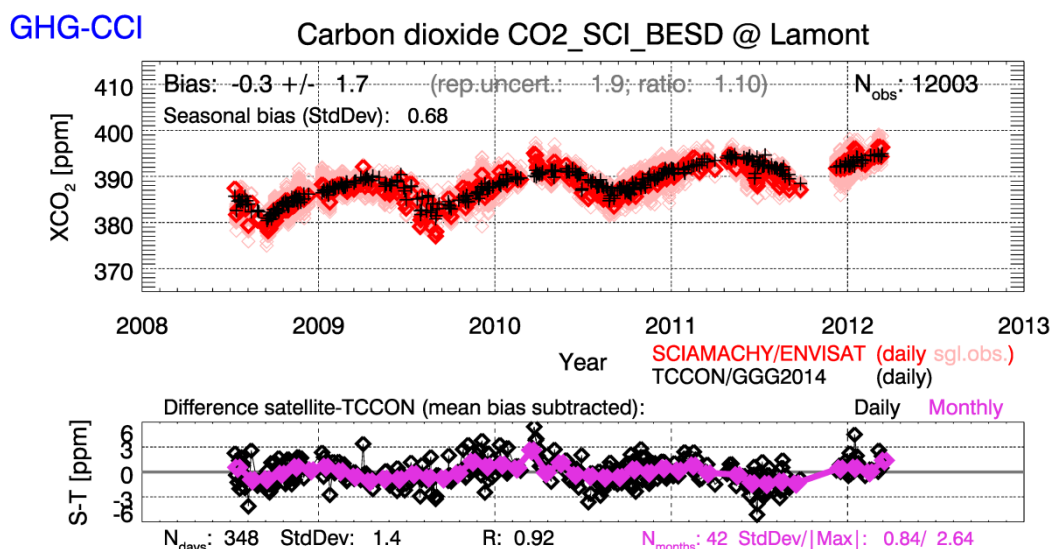
467 each individual ground pixel). This has been done by computing the ratio of the mean value of the

468 reported uncertainty to the standard deviation of the difference to TCCON. Figures such as Fig. 3 have

469 been generated for all ECA XCO<sub>2</sub> products and all selected TCCON sites (not shown). The most

470 important figures of merit for product CO2\_SCI\_BESD at all six TCCON sites are presented in Tab.

4. Table 4 also lists summary results (obtained by computing the sum, the mean and/or the standard deviation of the results obtained at the individual TCCON sites). The summary results for all four XCO<sub>2</sub> products are listed in Tab. 6.



**Figure 3:** Comparison of product CO<sub>2</sub>\_SCI\_BESD with TCCON XCO<sub>2</sub> at TCCON site Lamont, Oklahoma, USA. Top: Satellite XCO<sub>2</sub> in light red for the individual soundings, i.e., single observations (“slg. obs.”) and red for daily averages (co-location criterion: +/- 4 degrees, +/- 2 hours). TCCON XCO<sub>2</sub> is shown in black. Listed are several figures of merit: “Bias” (mean +/- standard deviation of the difference of the individual satellite retrievals and TCCON), “Seasonal bias” (standard deviation of differences for 3-month time periods), “Nobs” (number of individual satellite retrievals) and in grey the mean value of the reported uncertainty of the individual XCO<sub>2</sub> retrievals (“rep. uncert.”) and the “ratio” of the reported uncertainty and the standard deviation of the difference to TCCON. Bottom: XCO<sub>2</sub> difference at daily (black) and monthly (pink) resolution. The listed key figures of merit are also shown in Tab. 4 along with the corresponding values obtained at other TCCON sites.

**Table 6:** Overall TCCON comparison results for the GHG-CCI XCO<sub>2</sub> products. The results for product CO2\_SCI\_BESD have been obtained from Tab. 4 (the corresponding tables for the other three products are not shown here). “Systematic error” lists the regional and seasonal biases and, in brackets, a combined values ( $bias_{tot}$  (see Eq. (1)). “Uncertainty” is the mean value of the reported uncertainty and uncertainty ratio “UncRat” (in brackets) is defined as for Tab. 4. Also listed is the “Trend” (with 3-sigma uncertainty), “Offset” (the mean difference relative to all TCCON sites) and the number of satellite soundings (“Nobs”) compared to TCCON. At the bottom the corresponding requirements are listed based on GCOS, 2011, and on the GHG-CCI User Requirements Document (URD) (specified as Goal (G), Breakthrough (B) and Threshold (T)) (Chevallier et al., 2014b). Note that the GCOS requirements are target (maximum) requirements, whereas the URD threshold requirements are minimum requirements. The URD requirement for the systematic error is therefore much more demanding than the GCOS requirement but the stability requirements are identical. Note that the uncertainty of the TCCON reference data used to obtain the estimates listed here is about 0.4 ppm (1-sigma).

Product	Systematic error [ppm] Regional, seasonal (combined)	Uncertainty (Random error) [ppm] (UncRat)	Trend (Stability) [ppm/year]	Offset [ppm]	Nobs [-]
CO2_SCI_BESD	0.4, 0.8 (0.9)	1.9 (1.1)	-0.01 +/- 0.09	-0.2	26806
CO2_SCI_WFMD	0.6, 1.1 (1.3)	3.0 (1.1)	0.01 +/- 0.10	0.6	50087
CO2_GOS_OCFP	0.3, 0.5 (0.6)	1.7 (1.4)	-0.11 +/- 0.14	0.1	6139
CO2_GOS_SRFP	0.6, 0.5 (0.8)	1.9 (1.0)	-0.08 +/- 0.11	0.1	6795
<b>Required</b> <b>G / B / T</b>	< 1 < 0.2 / 0.3 / 0.5	- < 1 / 3 / 8	< 0.2 < 0.2 / 0.3 / 0.5	GCOS (2011) GHG-CCI URD (Chevallier et al., 2014b)	

As can be seen from Tab. 6, column “Systematic error”, the estimated regional bias of product CO2\_SCI\_BESD is 0.4 ppm and the estimated seasonal bias is 0.8 ppm. The regional bias has been estimated as standard deviation of the biases obtained at the individual TCCON sites (“station-to-station bias”) (see Tab. 4 for CO2\_SCI\_BESD). The seasonal bias is the mean value (over all TCCON sites) of the standard deviation of 3-monthly biases as obtained at the individual TCCON sites (see Dils et al., 2014, for a similar estimation of biases). The method of computing standard deviations neglects a possible overall offset relative to TCCON (listed separately in Tab. 6) but this is in line with the GHG-CCI User Requirements Document (URD, Chevallier et al., 2014b) which explains that spatio-temporal variations of biases are critical but overall (constant) offsets can be dealt with when using the satellite data products for inverse modelling (in other words “relative accuracy” is more important than “absolute accuracy”; note that in this manuscript the terms “accuracy”, “systematic error” and “bias” have the same meaning). Furthermore, a combined systematic error,  $bias_{tot}$ , is listed in column “Systematic error” in brackets, which has been computed from the regional and seasonal biases as follows:

$$bias_{tot} = \sqrt{bias_{reg}^2 + bias_{seas}^2} \quad \text{Eq. (1)}$$

As can be seen from Tab. 6, the biases of the other products are quite similar. All values are below 1 ppm except for product CO2\_SCI\_WFMD, where the total bias is 1.25 ppm. Tab. 6 also lists the required performance. As can be seen, all products (with the exception of CO2\_SCI\_WFMD, which has the advantage of providing the largest number of data points) meet the GCOS systematic error requirement (of better than 1 ppm) but not the much more demanding requirement as listed in the GHG-CCI URD (better than 0.5 ppm). However, as already mentioned above, one also has to consider the uncertainty of the TCCON retrievals (see also Buchwitz et al., 2015, for a discussion of this aspect). The systematic and random errors of single TCCON data are typically 0.4 ppm for XCO<sub>2</sub> (1-sigma) and 4 ppb (1-sigma) for XCH<sub>4</sub> (see Notholt et al., 2012, based on Wunch et al., 2010).

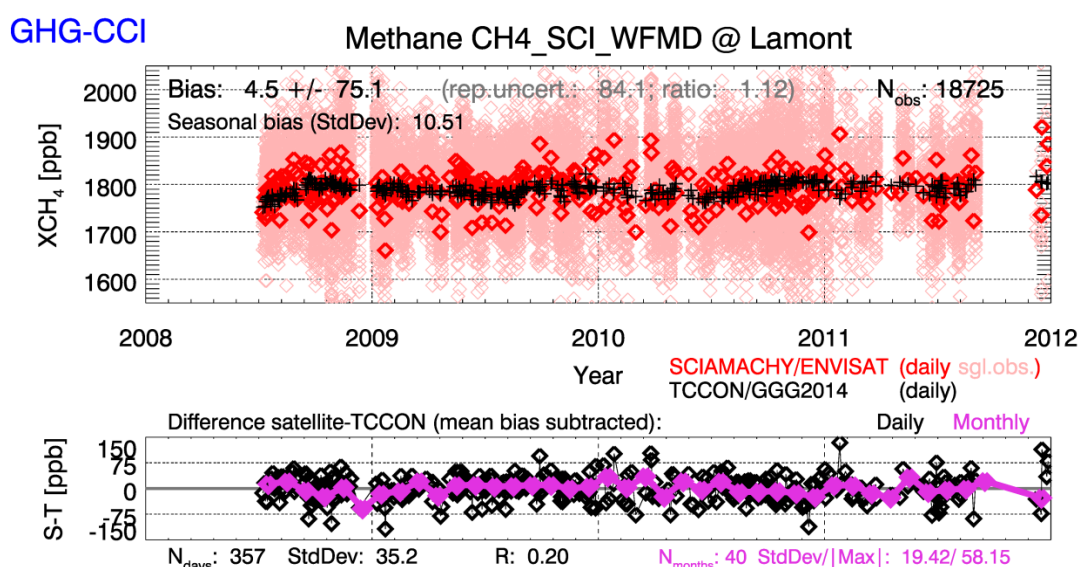
Assuming an overall TCCON bias uncertainty of 0.4 ppm for XCO<sub>2</sub> (see also Kulawik et al., 2016) and adding this (in a root-sum-square manner (e.g., Eq. (1)) to the 0.5 ppm URD requirement yields 0.64 ppm, i.e., a number somewhat larger than the overall bias for product CO2\_GOS\_OCFP (0.58 ppm). It is therefore possible that product CO2\_GOS\_OCFP even meets the demanding GHG-CCI URD threshold systematic error requirement of better than 0.5 ppm.

Table 6 also lists mean values of the reported uncertainty (essentially the random error component of the single ground pixel satellite retrievals) and the “uncertainty ratio“ (“UncRat”, in brackets), i.e., the ratio of reported uncertainty and standard deviation of the difference to TCCON. For the CO2\_SCI\_BESD product the reported uncertainty is 1.9 ppm (on average) and the uncertainty ratio is 1.1 providing confidence that the reported uncertainty is realistic (at least on average). This is also true for the other products with the exception of CO2\_GOS\_OCFP which appears to overestimate the uncertainty by about 40% on average, i.e., the reported uncertainty is quite conservative. As can also be seen, all products clearly meet the GHG-CCI URD breakthrough requirement of better than 3 ppm or are very close to meeting it (for product CO2\_SCI\_WFMD the estimated precision is 3.0 ppm).

Table 6 also lists the linear trend and its uncertainty, which has been determined by fitting a straight line to the individual satellite minus TCCON differences (after removal of a possible seasonal cycle obtained by fitting a linear combination of harmonics (sine and cosine functions) to the data). The trend uncertainty as given here is the 3-sigma uncertainty of the estimated trend. Assuming that only trends which are larger than their uncertainty are significant, one can see that none of the trends is significant. This indicates very good long-term stability (or, more precisely, the absence of a linear drift) of all satellite XCO<sub>2</sub> products (note that even the goal requirement of better than 0.2 ppm/year is met for all products).

### 3.2 XCH<sub>4</sub> comparisons with TCCON

Similar comparisons as presented in the previous sub-section have also been performed for the XCH<sub>4</sub> ECA products. Detailed example results for product CH<sub>4</sub>\_SCI\_WFMD are shown in Fig. 4 and Tab. 5. The most relevant figures of merit, defined as for XCO<sub>2</sub> (see previous section), are summarized along with the results for the other products in Tab. 7.



**Figure 4:** As Fig. 3 but for product CH<sub>4</sub>\_SCI\_WFMD.

As can be seen from Tab. 7, the (relative) biases are around 20 ppb for the SCIAMACHY products, which is worse than the required performance of better than 10 ppb. A much better performance in the range 6-7 ppb has been achieved for the GOSAT products (which, however, contain significantly less observations). The GOSAT products meet the GCOS and GHG-CCI URD systematic error (“accuracy”) requirements.

As can also be seen from Tab. 7, the GOSAT products also meet the GHG-CCI breakthrough requirement for random errors (better than 17 ppb) in contrast to the SCIAMACHY products which do

not meet the threshold requirement. However one has to point out that the first years of  
 SCIAMACHY, where the data quality is much higher, is under-represented here as no TCCON  
 observations are available during the first nearly two years of the ENVISAT mission (see Tab. 3).

**Table 7:** As Tab. 6 but for the GHG-CCI XCH<sub>4</sub> products. Note that the uncertainty of the TCCON  
 reference data used to obtain the estimates listed here is about 4 ppb (1-sigma).

<b>Product</b>	<b>Systematic error [ppb]  Regional, seasonal (combined)</b>	<b>Uncertainty (Random error) [ppb] (UncRat)</b>	<b>Trend (Stability)  [ppb/year]</b>	<b>Offset [ppb]</b>	<b>Nobs [-]</b>
CH4_SCI_WFMD	11.3, 16.8 (20.3)	81.6 (1.0)	2.0 +/- 4.3	-2.6	46958
CH4_SCI_IMAP	14.8, 14.4 (20.7)	48.3 (1.3)	4.5 +/- 2.8	-13.2	64841
CH4_GOS_OCPR	4.6, 3.4 (5.7)	11.9 (1.0)	0.0 +/- 1.1	6.5	14639
CH4_GOS_SRPR	3.4, 5.1 (6.1)	12.8 (0.9)	-0.9 +/- 1.0	-2.6	13502
CH4_GOS_SRFP	4.7, 5.1 (6.9)	12.6 (1.0)	-1.0 +/- 1.3	-1.4	6819
CH4_GOS_OCFP	4.1, 5.7 (7.0)	13.4 (0.7)	-0.4 +/- 1.2	0.7	5913
<b>Required</b>	< 10	-	< 2	GCOS (2011)	
<b>G / B / T</b>	< 1 / 5 / 10	< 9 / 17 / 34	< 1 / 5 / 10	GHG-CCI URD (Chevallier et al., 2014b)	

Table 7 also shows that the GOSAT products are very stable meeting the GCOS and (typically) even  
 the GHG-CCI URD goal requirement. The SCIAMACHY products do not meet the GCOS stability  
 requirement but apparently meet the GHG-CCI breakthrough requirement (of less than 5 ppb/year), at  
 least concerning linear long-term drifts. However we also looked at shorter-term drifts of biases and

identified issues in particular for the year 2010 and later years due to remaining issues from detector degradation (see Fig. 2).

#### 4. XCO<sub>2</sub> comparisons with global models

In the previous section we have presented validation results at selected TCCON sites. We have also performed detailed validation at a much larger number of TCCON sites as shown in Dils et al., 2016. Nevertheless, the number of ground-based validation sites is limited and large parts of the Earth are not covered (e.g., Africa, South America and large parts of Asia). Therefore, we present in this section detailed comparisons with global data sets (for recent comparisons with global models addressing different aspects see also Lindqvist et al., 2015, Parker et al., 2015, Kulawik et al., 2016). Here we use the output of the two global CO<sub>2</sub> assimilation systems (“models”) MACC (Chevallier et al., 2015), version 14r2, and CarbonTracker (Peters et al., 2007), version CT2013B. Note that comparisons with global models as well as CO<sub>2</sub> flux inversion results using CRDP3 XCO<sub>2</sub> (and XCH<sub>4</sub>) are also presented and discussed in Chevallier et al., 2016.

The European MACC (Monitoring of Atmospheric Composition Change) / CAMS (Copernicus Atmospheric Monitoring System) project global atmospheric CO<sub>2</sub> reanalysis data product, version v14r2, has been obtained from the MACC/CAMS website (<http://macc.copernicus-atmosphere.eu/catalogue/> -> <http://apps.ecmwf.int/datasets/data/macc-ghg-inversions/>, access: 23-Feb-2016). The MACC Bayesian inversion method (e.g., Chevallier et al., 2015, and references given therein) is formulated in a variational way in order to estimate CO<sub>2</sub> surface fluxes at relatively high resolution over the globe. Fluxes and mole fractions are linked in the system by the global atmospheric transport model of the Laboratoire de Météorologie Dynamique (LMDZ) with 39 layers in the vertical and with the same horizontal resolution than the inverted fluxes. LMDZ is nudged to ECMWF-analysed winds for flux inversion. The MACC inversion product also contains the 4-D CO<sub>2</sub> field that is associated to the inverted surface fluxes through the LMDZ transport model. These 4-D fields have been used for this study. Satellite XCO<sub>2</sub> observations have not been assimilated in MACCv14r2.

618

619 The CarbonTracker atmospheric CO<sub>2</sub> data product, version CT2013B, has been obtained from the  
620 NOAA/ESRL CarbonTracker website (<http://www.esrl.noaa.gov/gmd/ccgg/carbontracker/>, access: 3-  
621 Dec-2015) on which a detailed description of this version and how it has been generated is given. In  
622 short, CarbonTracker, developed by the National Oceanic and Atmospheric Administration (NOAA)  
623 Earth System Research Laboratory (ESRL), is an atmospheric CO<sub>2</sub> inverse modeling system that  
624 estimates optimized weekly surface CO<sub>2</sub> flux using the Ensemble Kalman Filter (EnKF) technique.  
625 Since the initial CarbonTracker release (Peters et al., 2007), a series of improvements have been made  
626 with subsequent releases. These include increasing the sites from which CO<sub>2</sub> data are assimilated,  
627 increasing the resolution of atmospheric transport, improving the simulation of atmospheric  
628 convection in the underlying transport model (TM5), and the use of multiple first-guess flux models to  
629 estimate dependence on priors. These improvements are documented at <http://carbontracker.noaa.gov>.  
630 CT2013B is a revision to the previous release (CT2013) and has the same time span, 2000-2012. For  
631 CT2013B the atmospheric transport model has been significantly improved. CT2013B assimilates CO<sub>2</sub>  
632 observations which are part of ESRL's new ObsPack data delivery system  
633 (<http://www.esrl.noaa.gov/gmd/ccgg/obspace/>, Masarie et al., 2014). Satellite XCO<sub>2</sub> observations have  
634 not been assimilated in CT2013B.

635

636 In the following we show comparisons of three GHG-CCI XCO<sub>2</sub> products with these two models in  
637 order to find out if it is possible to identify which of the model data sets compares best with the  
638 satellite data. The comparison has been done for the years 2010 and 2011 as these are the two years  
639 where the SCIAMACHY and GOSAT time series overlap.

640

641 Figure 5a shows comparisons of the GHG-CCI satellite-derived XCO<sub>2</sub> data products BESD, SRFP and  
642 OCFP with the MACC and CarbonTracker (CT) model data sets for the time period June-August  
643 (JJA) 2010 at a resolution of 2°x2°. The model data have been sampled according to the time and  
644 location of the (individual) satellite retrievals and the satellite averaging kernels have been applied to  
645 the model data to consider the altitude sensitivity of the satellite retrievals when computing XCO<sub>2</sub>

from the model CO<sub>2</sub> profiles (see Buchwitz et al., 2014). This has been done for each single satellite sounding (ground pixel) and afterwards the model data and the satellite data have been averaged (gridded 2°x2°) to obtain the maps shown in Fig. 5a.

The first row of Fig. 5a shows global maps of the three satellite data products. As can be seen, their spatial coverage differs. For example, the SCIAMACHY BESD data set is restricted to observations over land whereas the two GOSAT products also contain observations over oceans (corresponding to GOSAT sun-glint mode observations). As can also be seen, the spatial XCO<sub>2</sub> pattern over land show similarities but also differences. For example, all three products show elevated XCO<sub>2</sub> (red color) over similar parts of the western USA and Mexico, Amazonia and India and low XCO<sub>2</sub> over parts of eastern Russia but different patterns over Africa, in particular northern Africa. These differences could be a result of the different sampling (different spatio-temporal coverage) of the satellite data products within the JJA time period (due to differences of the SCIAMACHY and GOSAT overpass time and the different quality filtering procedures of the different retrieval algorithms).

To investigate the effect of spatio-temporal sampling one can compare the satellite retrievals with the model data sets. The middle row of Fig. 5a shows the MACC model sampled as the three satellite data products (e.g., the left panel in the middle row entitled MACC@CO<sub>2</sub>\_SCI\_BESD is the MACC model sampled as the BESD product). MACC sampled as the three satellite products (middle row) also shows elevated XCO<sub>2</sub> (red color) over similar parts of the western USA and Mexico, Amazonia and India in good to reasonable agreement with the satellite retrievals. Overall, all three MACC maps show similar XCO<sub>2</sub> pattern indicating that the pattern does not depend significantly on the sampling of the satellite data products. Over northern Africa MACC and OCFP show quite similar pattern whereas SRFP XCO<sub>2</sub> is significantly higher. There are nearly no BESD data over northern Africa as most of the BESD retrievals have been removed by the very strict BESD quality filter.

The bottom row of Fig. 5a shows CT sampled as the three satellite data products. Overall, there is good agreement between CT and MACC but there are also differences. For example, CT shows

significantly lower XCO<sub>2</sub> over large parts of eastern Russia compared to MACC. The satellite products show XCO<sub>2</sub> values which are in between the values of MACC and CT but are significantly closer to MACC (see also Fig. 5b discussed below). This may indicate that over eastern Russia the CT XCO<sub>2</sub> is somewhat too low during summer (JJA season; note that we get similar comparison results also for JJA 2011 not shown here).

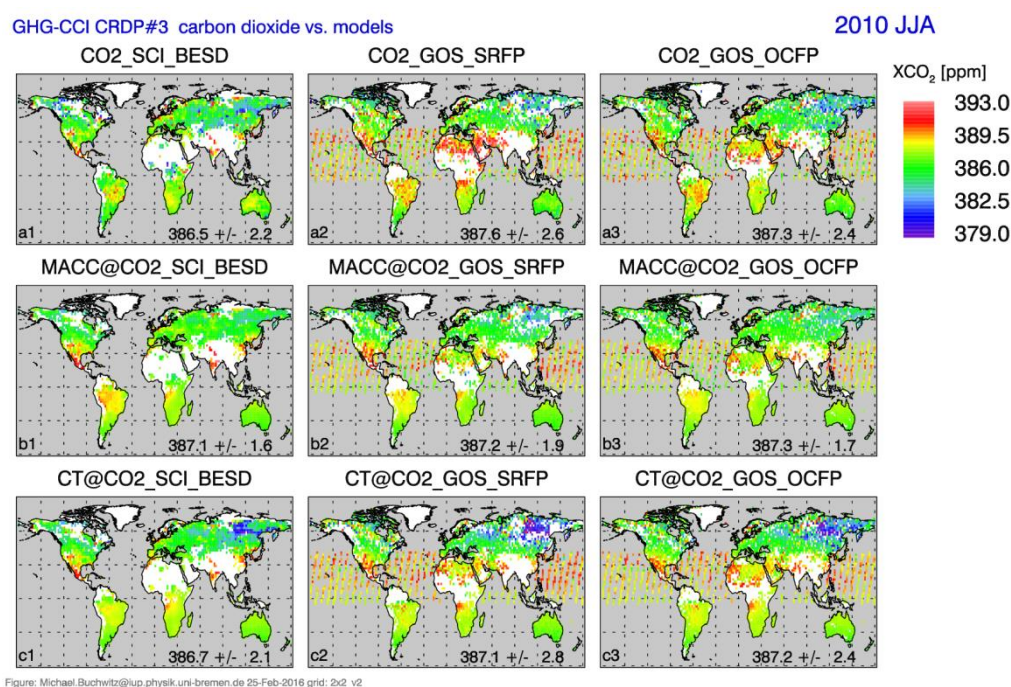
Figure 5b shows the differences between the models and the satellite data (first two rows) and the difference between the two models (bottom row). The bottom row shows that the largest difference between the two models is over large parts of eastern Russia with differences up to about +4 ppm (MACC higher than CT). For other regions the agreement is mostly in the range +/-2 ppm (green color). As can also be seen, the satellite data are in better agreement with MACC over eastern Russia.

To also consider the uncertainty of the satellite retrievals we have generated Fig. 5c. Our estimated uncertainties are shown in the bottom row of Fig. 5c. These uncertainties ( $unc_{tot}$ ) have been computed as follows:

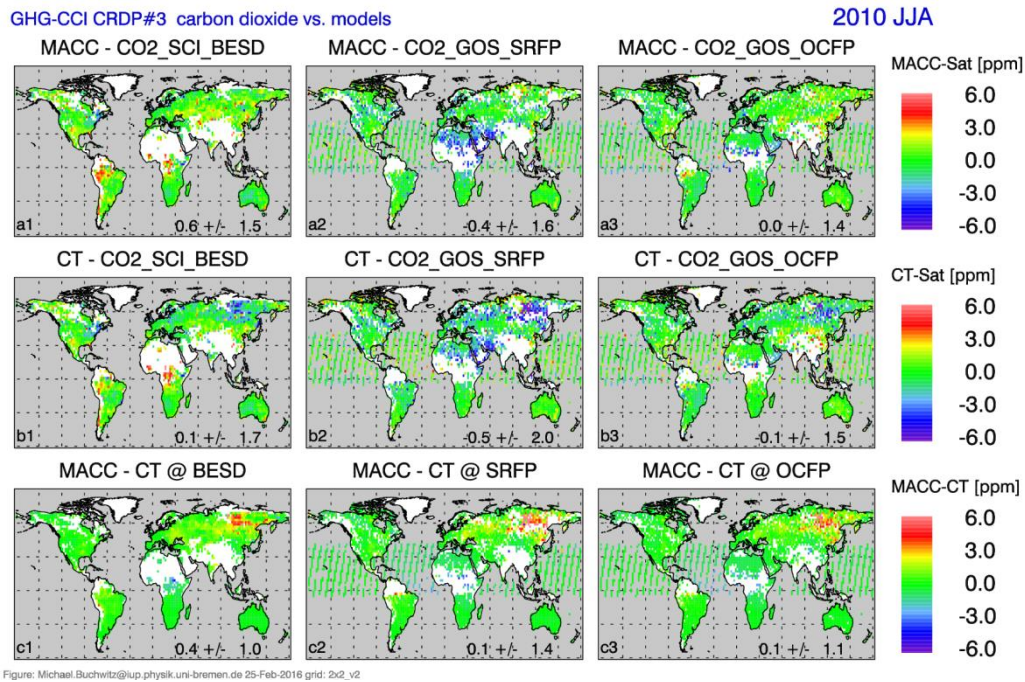
$$unc_{tot}(N) = \sqrt{bias_{tot}^2 + \frac{rnd^2}{N}} \quad \text{Eq. (2)}$$

Here  $N$  are the number of satellite retrievals per (2°x2°) grid cell,  $bias_{tot}$  is the systematic error component of the total uncertainty (see Eq. (1) and Tab. 6) and  $rnd$  is the random error component of the total uncertainty for single observations, which is assumed here to improve with  $\sqrt{N}$  when  $N$  observations are averaged (see also Kulawik et al., 2016, and Sect. 5 for an assessment of how SCIAMACHY and GOSAT XCO<sub>2</sub> uncertainties depend on the number of observations added).  $rnd$  has been computed by averaging the reported uncertainties of the  $N$  XCO<sub>2</sub> retrievals located in each grid cell. Here the reported uncertainties of the CO2\_GOS\_OCFP product have been divided by 1.4 to compensate for the approximately 40% overestimation of the reported errors (see previous discussion of the results presented in Tab. 6). As can be seen from the bottom row of Fig. 5c, the uncertainty of the three satellite data products is typically around 1.2 ppm (standard deviation 0.5 ppm).

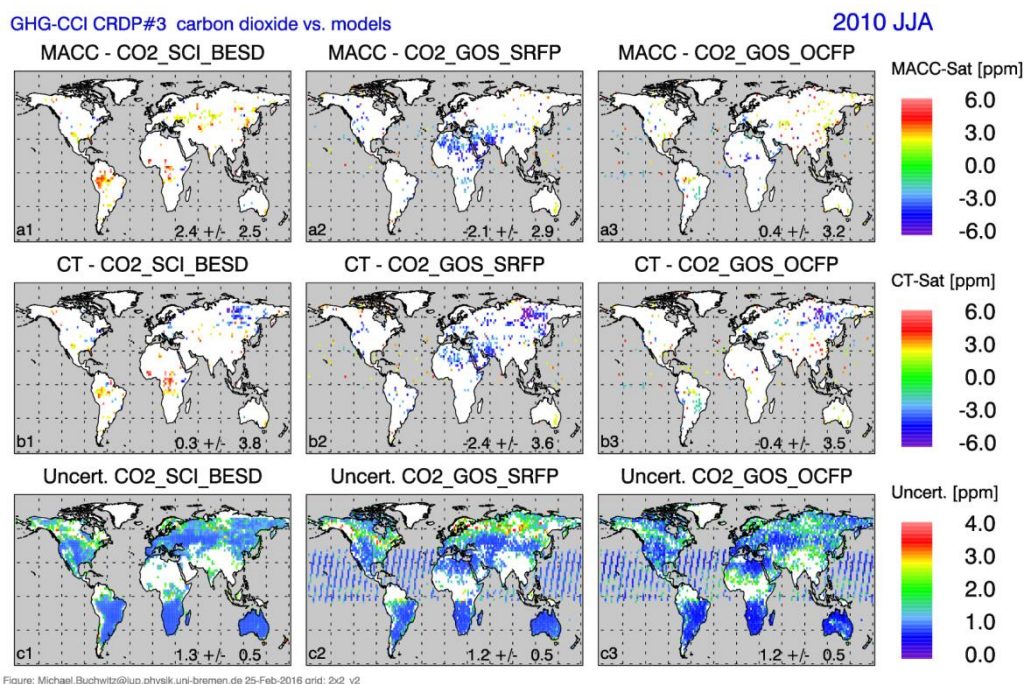
The first two rows displayed in Fig. 5c show the same model minus satellite differences as also shown in Fig. 5b but restricted to those ( $2^\circ \times 2^\circ$ ) grid cells where the (absolute value of the) difference is larger than the uncertainty shown in the bottom row, i.e., the first two rows only show cells with likely “significant differences”. As can be seen, OCFP shows hardly any significant differences at least for extended regions (of connected cells). An exception is the already discussed part of eastern Russia, where differences are significant for CT (for all three satellite products) but not for MACC. Over parts of Amazonia MACC XCO<sub>2</sub> is higher than BESD but this difference is much smaller for CT. Over parts of central Africa both models are higher than BESD. SRFP shows extended regions of differences over parts of northern Africa, Saudi Arabia and Iran (SRFP higher than the models as already mentioned when discussing Fig. 5a).



**Figure 5a:** Top: Satellite XCO<sub>2</sub> gridded  $2^\circ \times 2^\circ$  for June-August 2010 for the three products BESD (left), SRFP (middle) and OCFP (right). Middle: MACC XCO<sub>2</sub> sampled as the three satellite products. Bottom: CarbonTracker sampled as the satellite products.

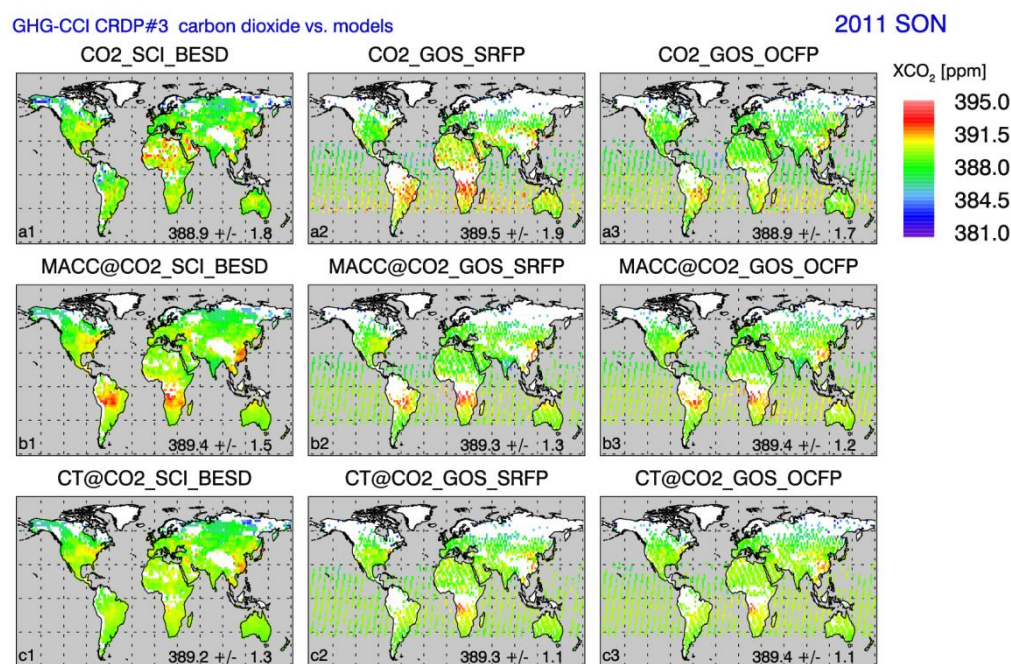


**Figure 5b:** As Fig. 5a but for the difference MACC-satellite (top), CarbonTracker-satellite (middle) and MACC-CarbonTracker (bottom) sampled according to the three satellite products BESD (left), SRFP (middle) and OCFP (right).



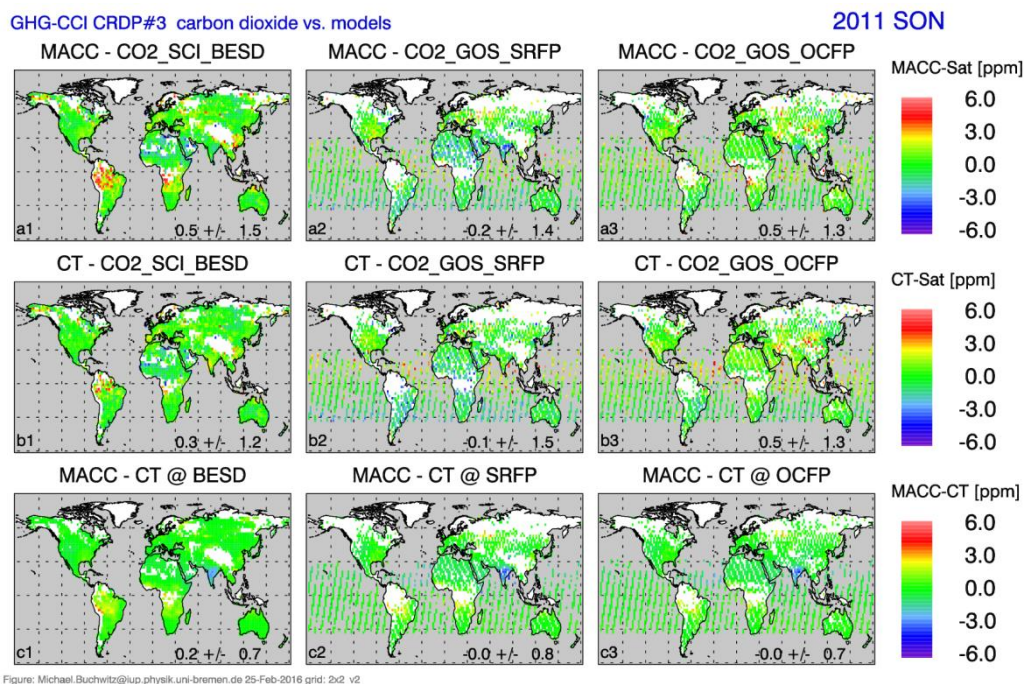
**Figure 5c:** As Fig. 5b but only for “significant” satellite-model differences (top and middle row) obtained by considering the uncertainty of the satellite retrievals (bottom). See main text for details.

Figures 6a – 6c show the same maps as Figs. 5a – 5c but for the time period September – November 2011. Here the models show differences in particular over parts of Amazonia, southern Africa and India (Figs. 6a) of about 2-3 ppm (Figs. 6b, bottom). The “significant differences” between the models and the satellite retrievals are shown in Figs. 6c (top row for MACC; middle row for CT). Over Amazonia and parts of southern Africa MACC is higher than BESD over large regions, whereas CT shows less differences to BESD over Amazonia and hardly any differences over southern Africa. For southern Africa the differences between the models and BESD are similar as for OCFP. Over Africa both models are lower compared to SRFP. Over India both models, MACC and CT, are lower than SRFP and OCFP.



**Figure 6a:** As Fig. 5a but for September–November 2011.

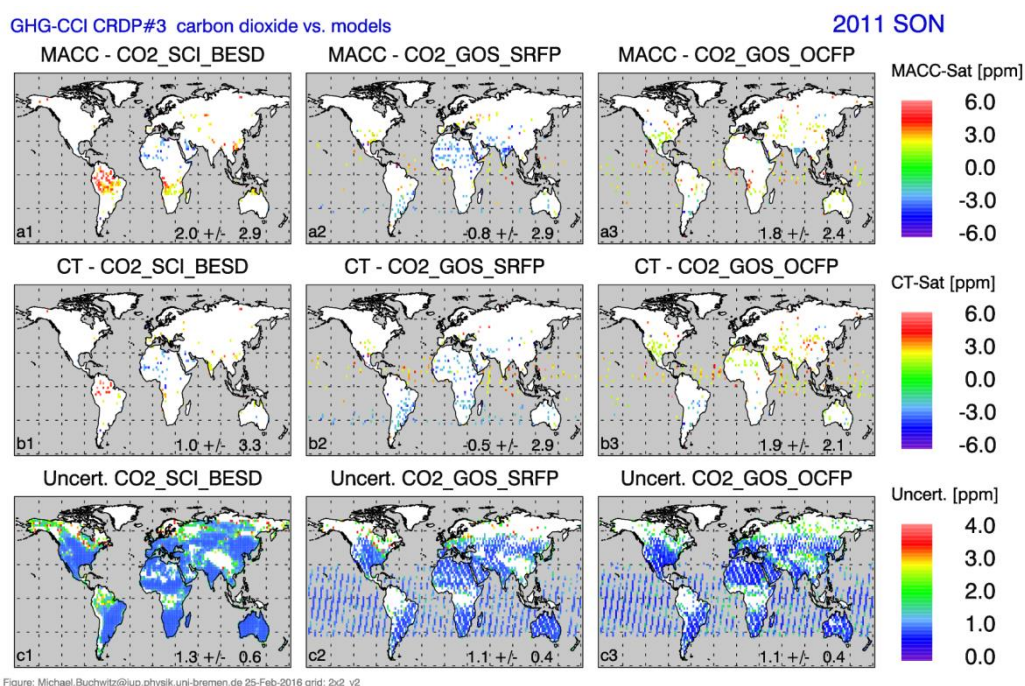
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739

740 **Figure 6b:** As Fig. 5b but for September-November 2011.

741



742

743 **Figure 6c:** As Fig. 5c but for September-November 2011.

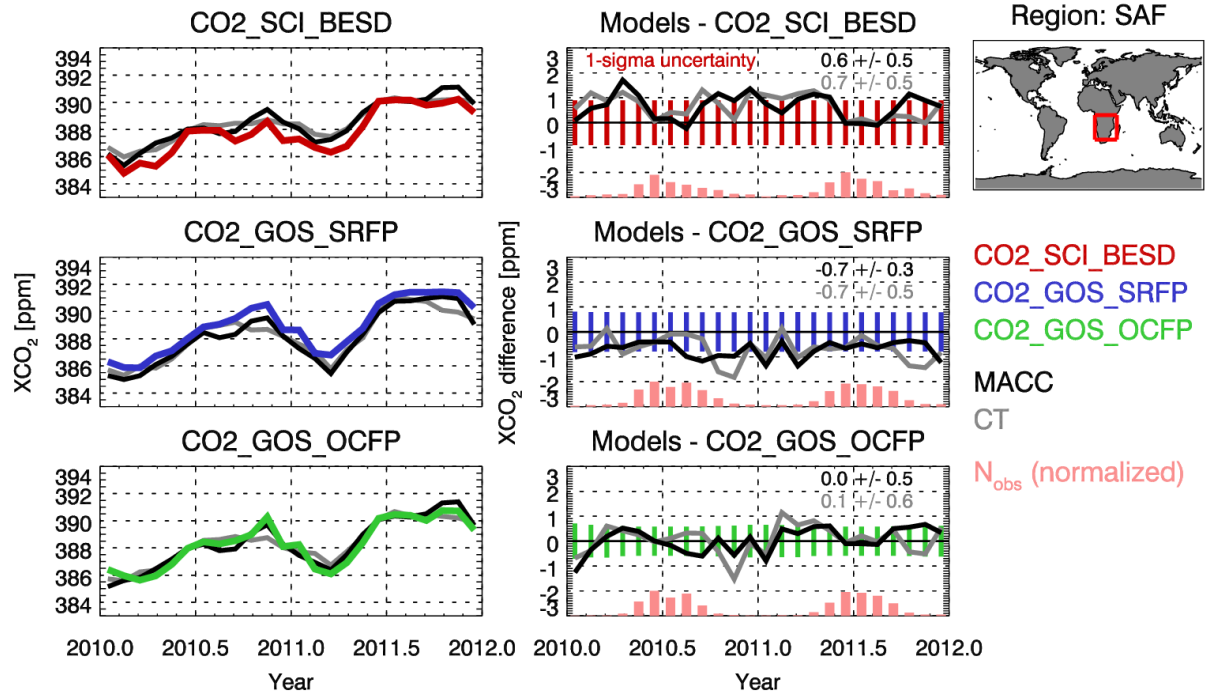
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745

To further investigate the agreements / disagreements between the XCO<sub>2</sub> data sets we also generated time series. Figures 7 – 11 show time series of the satellite and model data sets for some of the discussed regions but also for other regions. Figure 7 shows time series for the region southern Africa (SAF) based on monthly averages. The top left panel shows BESD XCO<sub>2</sub> (in red), MACC (black) and CT (grey) sampled as BESD. The panel on the right next to that panel shows the model – BESD differences as solid lines (in black for MACC and grey for CT) but also the estimated uncertainty (1-sigma) of the satellite data (red vertical bars, one for each month). As can be seen, both models are higher by about 0.6 ppm compared to BESD (top row), lower by about 0.7 ppm compared to SRFP (middle), whereas the average difference is close to zero for OCFP. The standard deviation of the monthly differences is 0.5 ppm for BESD for both models, for SRFP 0.3 ppm relative to MACC and 0.5 ppm relative to CT, and for OCFP 0.5 ppm relative to MACC and 0.6 ppm relative to CT. Note that typically the agreement between the models and the satellite retrievals is best where the number of satellite observations is highest (see N<sub>obs</sub> bars in light red). Overall, OCFP shows the best agreement with the two models with most of the differences within 1 ppm.

Figs. 8 - 11 also show time series as Fig. 7 but for the regions northern Africa (NAF, Fig. 8). North America (NAM, Fig. 9), Europe (EUR, Fig. 10) and China (CHI, Fig. 11). For region NAF (Fig. 8), BESD and OCFP agree with the models within typically 1 ppm whereas SRFP has an apparent high bias of around 1.4 ppm. For region NAM (Fig. 9) the situation is similar for BESD and OCFP but the agreement is better for SRFP. For Europe (Fig. 10) the two models agree with each other but show typically a high bias compared to the satellite retrievals. For China (Fig. 11) the models typically agree with SRFP and OCFP within 1 ppm whereas the comparison with BESD shows somewhat larger differences for some months.

## GHG-CCI CRDP#3 carbon dioxide

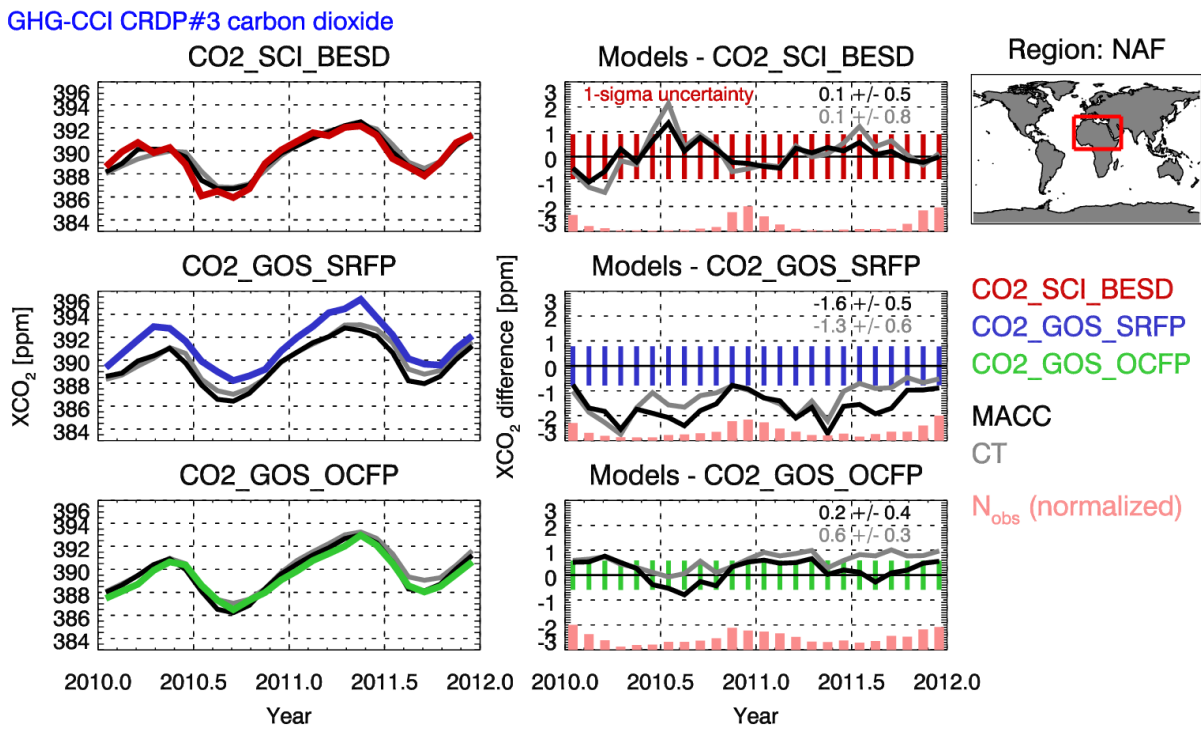


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**Figure 7:** Timeseries of satellite and model XCO<sub>2</sub> for region Southern Africa (SAF; see map top right). Top left: Monthly XCO<sub>2</sub> BESD (red), MACC XCO<sub>2</sub> sampled as BESD (black) and CarbonTracker XCO<sub>2</sub> sampled as BESD (grey). Top middle: models – satellite for BESD: MACC-BESD (black) and CarbonTracker-BESD (grey). The red vertical bars indicate the estimated uncertainty of the satellite retrievals. In light red the number of satellite observations per month is shown (in arbitrary units). Middle: as top row but for SRFP (blue), Bottom: as top and middle row but for OCFP (green). Listed on top right in each panel on the right hand side is mean +/- standard deviation of the difference between the models and the satellite XCO<sub>2</sub>.

Overall it can be concluded that the models agree with the satellite retrievals within typically 1-2 ppm but depending on region and time period differences can also be somewhat larger. As shown in Kulawik et al., 2016, MACC and CT fit TCCON typically quite well but TCCON stations are usually in place where there are surface air sample measurements to constrain the models (see also Parker et al., 2015). Differences may therefore be larger elsewhere. Nevertheless, we found that the two model data sets are very similar, in particular when averaged over large region (see regional timeseries).

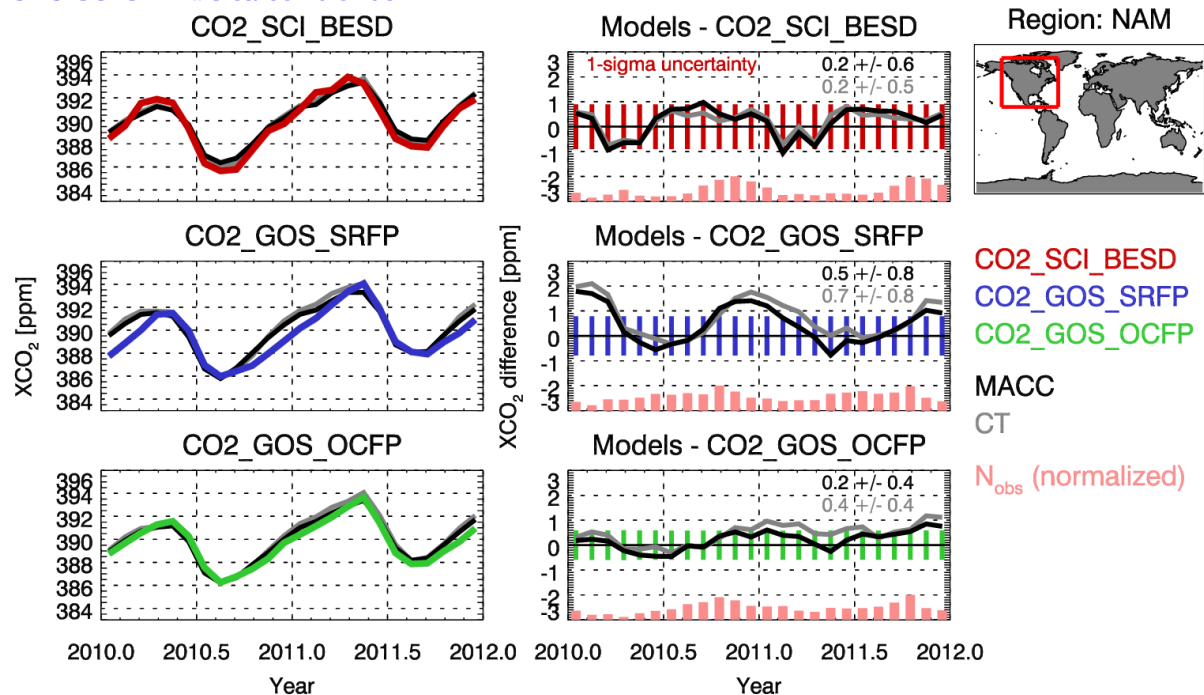
However, we also identified significant differences between them. For example, CT shows significantly lower  $XCO_2$  compared to MACC (approximately 4 ppm) over large parts of eastern Russia during summer 2010 (JJA season) (also during JJA 2011, but this has not been shown here). Over parts of Amazonia and southern Africa during autumn 2011 (SON season) MACC is about 2 ppm higher than CT and over India MACC is about 2-3 ppm lower (also for SON 2010, not shown here). We also identified significant differences between the satellite data products, e.g., a high or a low bias of SRFP compared to the other two satellite products BESD and OCFP depending on region and time period.



**Figure 8:** As Fig. 7 but for region Northern Africa (NAF).

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GHG-CCI CRDP#3 carbon dioxide



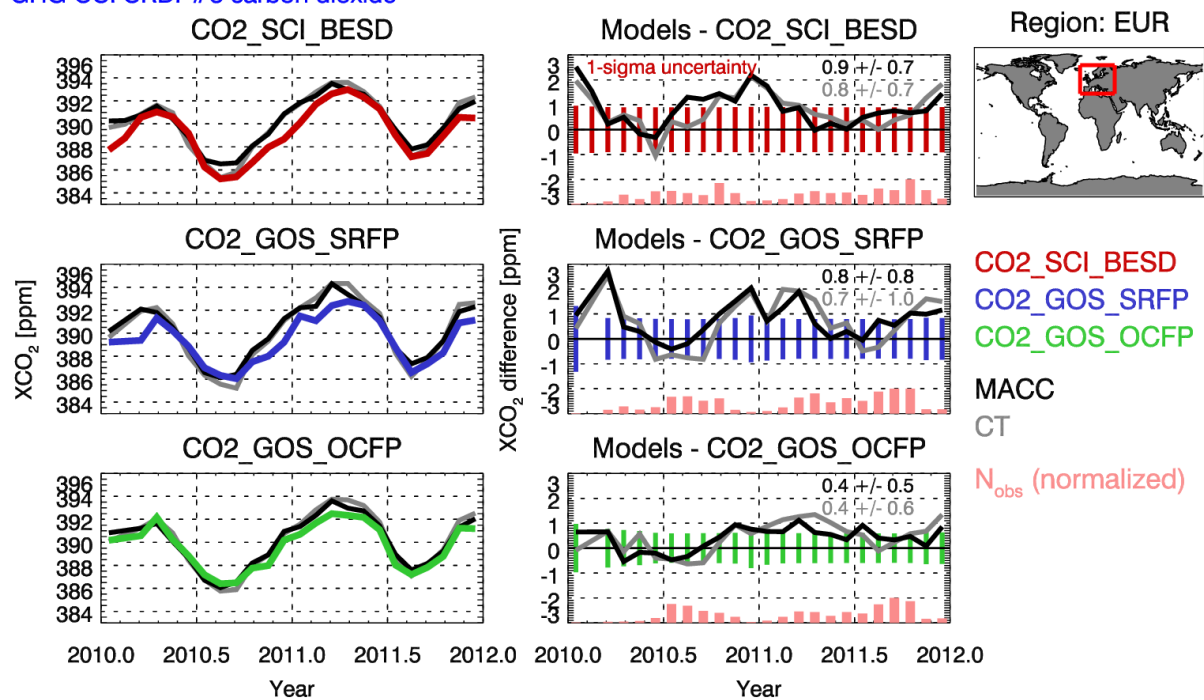
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803 **Figure 9:** As Fig. 7 but for region North America (NAM).

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GHG-CCI CRDP#3 carbon dioxide

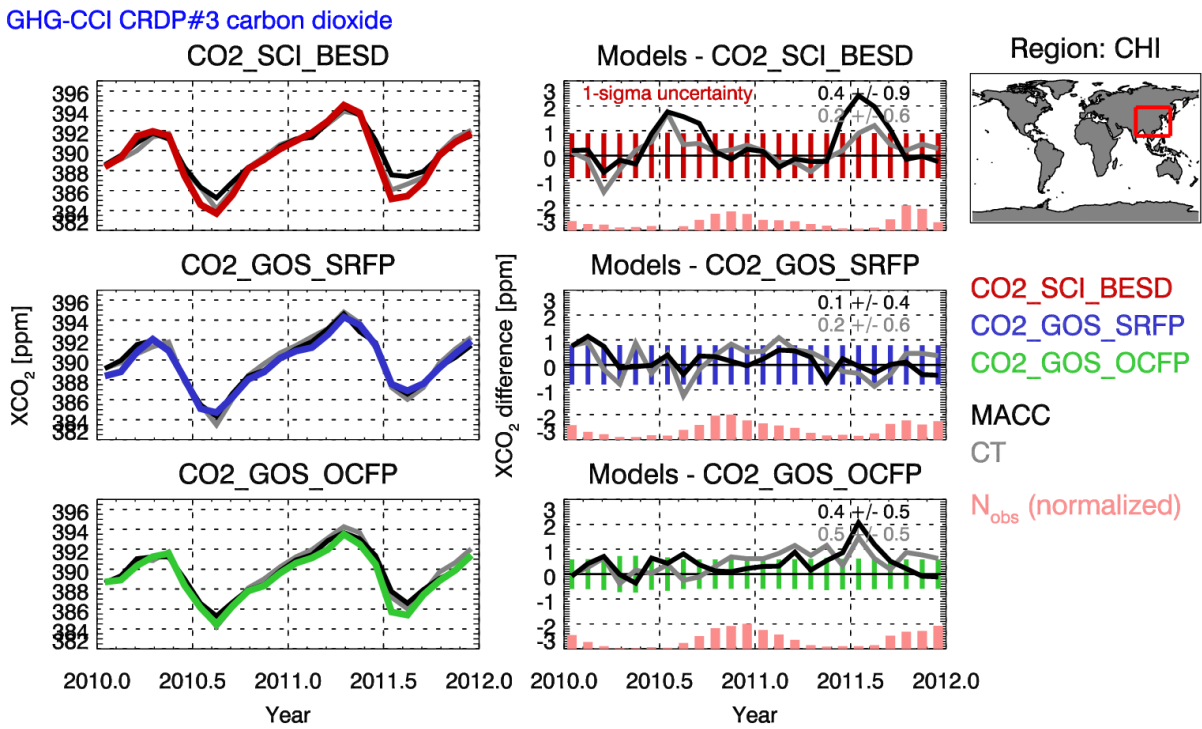


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806 **Figure 10:** As Fig. 7 but for region Europe (EUR).

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**Figure 11:** As Fig. 7 but for region China (CHI).

## 5. XCO<sub>2</sub> error correlations

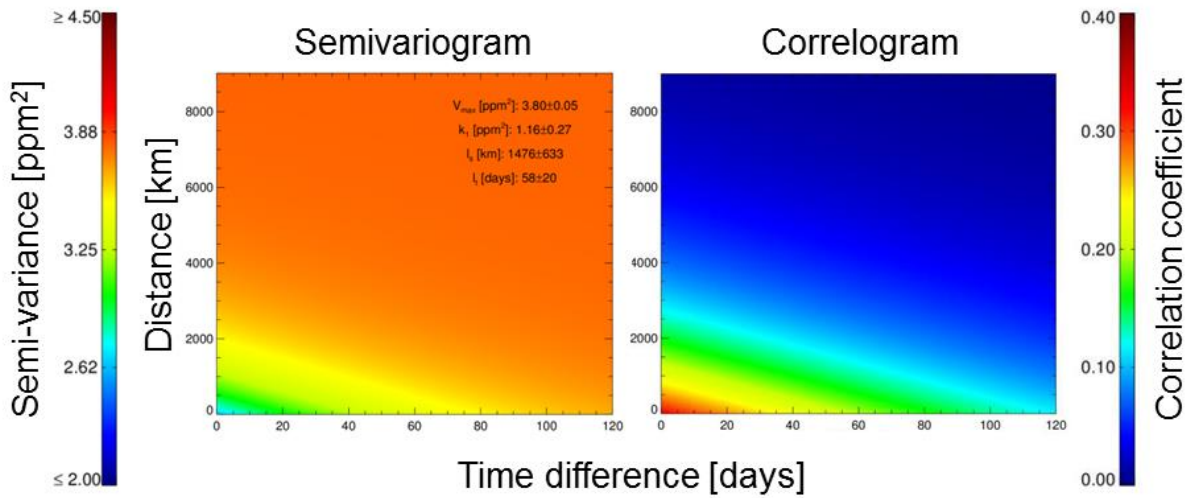
The GHG-CCI ECA products are Level 2 products, i.e., product information such as XCO<sub>2</sub> and its uncertainty is reported for each individual satellite ground pixel. For applications such as inverse modelling also information on spatio-temporal error correlations would be highly beneficial (see Chevallier et al., 2014b). However, it is not trivial because the needed co-located ground truth observations are only available at TCCON sites, which makes it difficult to obtain reliable global statistics representative for all temporal and spatial distances. Additionally, error correlations may systematically differ depending on surface reflectivity, atmospheric composition (e.g., aerosols and cirrus), viewing geometry and solar illumination conditions. This would violate the assumption of stationarity made by our approach.

Here we report on an attempt to obtain spatio-temporal error correlations in a form useful for inverse modelling and related applications such as CCDAS (Carbon Cycle Data Assimilation Systems (e.g., Kaminski et al., 2013)) (for alternative attempts see Chevallier et al., 2013, and Kulawik et al., 2016). The goal is to obtain a covariance matrix, where each diagonal element corresponds to the variance of the retrieved XCO<sub>2</sub> of a corresponding ground pixel, which is the square of the reported XCO<sub>2</sub> uncertainty, and each non-diagonal element corresponds to the co-variance between two retrievals, i.e., different ground pixels. Our method to estimate co-variances is based on semivariogram analysis (Montero et al., 2015) of the satellite minus TCCON XCO<sub>2</sub> differences. As shown in Reuter et al., 2016, where the analysis method is described in detail, we have used two different parameterizations resulting in a “full” and an “approximate” error covariance matrix. The full error covariance matrix (not shown here; see Reuter et al., 2016, for details) is dense and does not necessarily vanish even for long distances. Therefore, it may be computationally too expensive for many users. A simpler parametrization of the error covariance, whose use can be computationally less demanding, is given by the following formula (“exponential product model”):

$$C_{ij} = \frac{\sigma_i \sigma_j}{V_{max}} \begin{cases} k e^{-(\Delta s/l_s + \Delta t/l_t)}, & \Delta s > 0 \text{ or } \Delta t > 0 \\ V_{max}, & \Delta s = 0 \text{ and } \Delta t = 0 \end{cases} \quad \text{Eq. (3)}$$

Here,  $\sigma_i$  and  $\sigma_j$  correspond to the reported uncertainties for ground pixels  $i$  and  $j$  and  $\Delta s$  and  $\Delta t$  are their corresponding spatial (in km) and temporal (in days) differences, respectively. These uncertainties  $\sigma$  are related to the uncertainties reported in the BESDv02.01.01 product files,  $\tilde{\sigma}$ , by  $\sigma = \tilde{\sigma} * 0.2741 + 1.3294$  ppm.  $V_{max}$ ,  $k$ ,  $l_s$  and  $l_t$  are parameters obtained via model semivariogram least squares fitting. Parameter  $V_{max}$  (in semivariogram analyses often called “sill”, see, e.g., the textbook of Montero et al., 2015) corresponds to the error variance due to all error components. Parameter  $k$  is the variance due to correlated errors. The difference  $V_{max} - k$  (in semivariogram analyses often called “nugget”, see, e.g., the textbook of Montero et al., 2015) corresponds to the fully uncorrelated part of the error, e.g., due to instrumental noise. Parameter  $l_s$  is the spatial correlation length and  $l_t$  is the temporal correlation length. As shown in Reuter et al., 2016, the following values have been obtained for the

CO2\_SCI\_BESD product:  $V_{max} = 3.80 \pm 0.05 \text{ ppm}^2$ ;  $k = 1.16 \pm 0.27 \text{ ppm}^2$ ;  $l_s = 1476 \pm 633 \text{ km}$  and  $l_t = 58 \pm 20 \text{ days}$  (see Fig. 12). Equation 3 and its corresponding parameters has been derived based on relatively coarse assumptions (see Reuter et al., 2016, for details) and future analysis may result in a better approximation but for now we recommend that users who would like to or have to take error correlations into account use the results presented here.



**Figure 12:** Modelled semivariogram (left; with the four fit parameters listed top right) and corresponding correlogram (right) for product CO2\_SCI\_BESD. The correlogram,  $\rho$ , has been obtained from the semivariogram,  $\gamma$ , via  $\rho = 1 - \gamma/V_{max}$ . The covariance matrix,  $C$  (see Eq. (3)), and the correlogram,  $\rho$ , are related by  $\rho = C/V_{max}$ .

## 6. XCH<sub>4</sub> global maps and time series

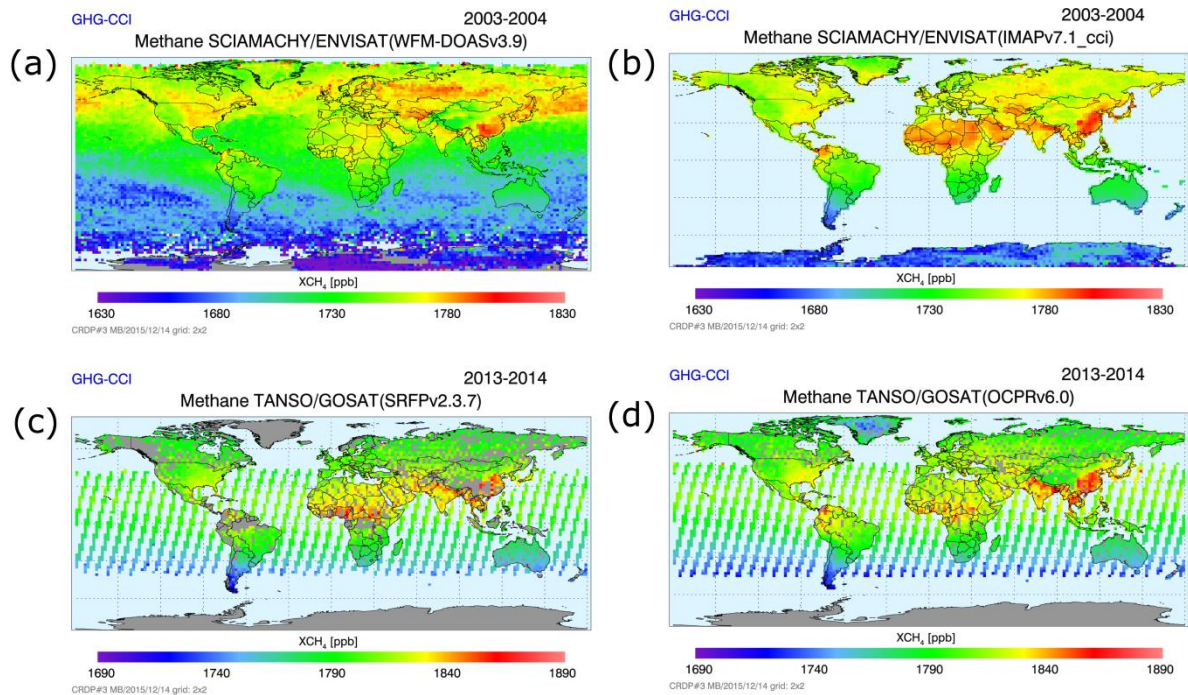
Finally we present some comparisons of global maps of XCH<sub>4</sub> ECA products (Figs. 13a – 13d). Note that many detailed figures for each month and each product (including number of observations per grid cell, standard deviation, etc.) and latitude-resolved time series for the CRDP3 products are shown on the GHG-CCI website (see XCH<sub>4</sub> (and XCO<sub>2</sub>) CRDP3 “browse images” on <http://www.esa-ghg->

[cci.org/](http://www.esa-ghg-cci.org/)) and detailed assessment results are presented in several technical documents (e.g., Buchwitz et al., 2016).

Figure 13a shows a global composite map of product CH<sub>4</sub>\_SCI\_WFMD for the years 2003-2004, i.e., for the first two years of the GHG-CCI ECA time series at 2°x2° resolution. A major feature is the north-south methane gradient, with higher concentrations over the northern hemisphere, where most of the methane sources are located. Clearly visible by higher regional XCH<sub>4</sub> values are major methane source regions such as China (wetland and rice paddy emissions). However, we have to point out that it is not trivial (if not impossible) to draw clear conclusions with respect to regional emissions from maps such as those shown in Fig 13a due to temporal sampling issues (depending on month, the satellite data may be quite sparse) combined with atmospheric transport and the long lifetime of CH<sub>4</sub> in the atmosphere. For example, large values over water (Fig. 13a) are typically not due to local sources but due to outflow from major source regions (e.g., Asia) located on land.

Figure 13b shows the corresponding map for product CH<sub>4</sub>\_SCI\_IMAP. As can be seen, this product is limited to observations over land. The spatial XCH<sub>4</sub> pattern is similar compared to WFMD (Fig. 13a) but not identical. This is due to differences in spatio-temporal sampling of the satellite data, different random errors (see Tab. 7), differences in altitude sensitivity but also due to (different) biases in the satellite data products.

Figures 13c and 13d show global maps for the two GOSAT products CH<sub>4</sub>\_GOS\_SRFP (Fig. 13c) and CH<sub>4</sub>\_SCI\_OCPR (Fig. 13d) for 2013-2014, i.e., for the two last years of the CRDP3 ECA data set. Both products show similar (but not identical) coverage and pattern, for similar reasons as explained above for the two SCIAMACHY products. Note that detailed comparison and assessment results are shown in Buchwitz et al., 2016, and other technical documents available on the GHG-CCI website (<http://www.esa-ghg-cci.org/>) and we recommend that users interested in these data products take the information given in these documents into account when using our data products for any given application.



**Figure 13:** Global maps of satellite-derived XCH<sub>4</sub>. (a) Global map of product CH<sub>4</sub>\_SCI\_WFMD obtained by gridding all individual retrievals during 2003-2004 using 2°x2° grid cells. (b) As (a) but for product CH<sub>4</sub>\_SCI\_IMAP. (c) As (a) but for CH<sub>4</sub>\_GOS\_SRFP during 2013-2014. (d) As (c) but for CH<sub>4</sub>\_GOS\_OCPR. Note the change of the color scale (+ 60 ppb) for the 2013-2014 maps, i.e., for (c) and (d).

## 7. Summary and conclusions

CO<sub>2</sub> and CH<sub>4</sub> are the two most important greenhouse gases emitted by mankind and responsible for a large fraction of the observed global warming. Despite their importance our knowledge on their various variable surface sources and sinks has significant gaps. Satellite observations of atmospheric CO<sub>2</sub> and CH<sub>4</sub> are increasingly being used to help closing relevant knowledge gaps. We have presented a short overview based on peer-reviewed publications to demonstrate the progress which has been made in recent years concerning the use of satellite retrievals of near-surface-sensitive column-averaged dry air mole fractions of CO<sub>2</sub> and CH<sub>4</sub>, i.e., XCO<sub>2</sub> and XCH<sub>4</sub>. Nevertheless, much more still

needs to be learned about the sources and sinks of these greenhouse gases but this requires additional efforts in terms of further improving the quality of the satellite retrievals, to extend their time series (using existing and future sensors) and to further improve transport modelling and inversion methods as well as more and better satellite and non-satellite observations (e.g., Ciais et al., 2014).

Here we have presented a new XCO<sub>2</sub> and XCH<sub>4</sub> satellite-derived data set called “Climate Research Data Package” No. 3 (CRDP3) which has been generated within the ESA CCI project GHG-CCI. The data products are available for all interested users from the website of this project (<http://www.esa-ghg-cci.org/>).

The presented XCO<sub>2</sub> and XCH<sub>4</sub> data sets cover the time period end of 2002 – 2014 and have been derived from the nadir near-infrared / shortwave-infrared (NIR/SWIR) radiance observations of the two satellite instruments SCIAMACHY/ENVISAT (2002 - 2012) and TANSO/GOSAT (launched 2009). We have presented time series and global maps including comparisons with TCCON (Wunch et al., 2010, 2011) ground-based observations (version GGG2014) and global CO<sub>2</sub> assimilation system (“models”) data sets (European MACC/CAMS model (v14r2) (Chevallier et al., 2015) and NOAA’s CarbonTracker (version CT2013B) (Peters et al., 2007)).

Based on validation using TCCON data at six sites we have shown that with one exception the satellite XCO<sub>2</sub> products have (relative) systematic errors of less than 1 ppm, i.e., they meet the Global Climate Observing System (GCOS) accuracy requirement. All XCO<sub>2</sub> products are very stable showing no significant long-term linear trend and they meet the GCOS stability requirement of better than 0.2 ppm/year.

The GOSAT XCH<sub>4</sub> retrievals also meet the GCOS accuracy requirement of better than 10 ppb and are even close to meeting the GHG-CCI breakthrough requirement of better than 5 ppb. These products are also very stable showing no significant long-term linear trend and they meet the GCOS stability requirement of better than 2 ppb/year. For the SCIAMACHY XCH<sub>4</sub> products the situation is more

complex due to detector degradation. In particular for 2010 and later years this results in significant biases (not meeting the GCOS accuracy requirement of better than 10 ppb) and large scatter.

The SCIAMACHY BESD XCO<sub>2</sub> and the two GOSAT XCO<sub>2</sub> products (SRON/KIT's SRFP ("RemoTeC")) product and University of Leicester's OCFP product) have been compared with output from the MACC model and NOAA's CarbonTracker (CT). Detailed comparison results are presented in terms of global maps and time series for selected regions. Overall it can be concluded that the CO<sub>2</sub> models agree with the satellite retrievals within typically 1-2 ppm but depending on region and time period differences can also be somewhat larger. The two model data sets are very similar, in particular when averaged over large regions, but we also identified significant differences between them. For example, CT shows significantly lower XCO<sub>2</sub> compared to MACC (approximately 4 ppm) over large parts of eastern Russia during summer (JJA season) with MACC being in better agreement with the satellite data compared to CT. Over parts of Amazonia and southern Africa during autumn (SON season) MACC is about 2 ppm higher than CT and over India MACC is about 2-3 ppm lower. For India the satellite data are in better agreement with CT compared to MACC but for Amazonia and southern Africa the situation is less clear. We also identified significant differences between the satellite data products, e.g., a high or a low bias of SRFP compared to other satellite products depending on region and time period. Because the link between atmospheric concentrations and surface fluxes is typically complex our analysis does not necessarily permit to draw clear conclusions on which satellite data set gives the most reliable surface fluxes when used in an inverse modelling framework. This underlines the importance of using multiple satellite products and inversion methods in order to draw robust conclusions on GHG sources and sinks as aimed at in several recent publications (e.g., Chevallier et al., 2013, 2016; Reuter et al., 2014a; Houweling et al., 2015; Feng et al., 2016).

Furthermore, we have presented an attempt to provide users with information on spatio-temporal error correlations using a parameterization of an error covariance matrix obtained via semivariogram analysis of satellite minus TCCON XCO<sub>2</sub> differences. We have also presented global XCH<sub>4</sub> maps to

illustrate how the various new XCH<sub>4</sub> products “look like”. Finally, we would like to point out that additional information in terms of various technical documents and separate figures is available on the website of the GHG-CCI project (<http://www.esa-ghg-cci.org/>) (please note in particular the link to “CRDP (Data)”).

## Acknowledgements

This study has been funded by ESA via the GHG-CCI project of ESA’s Climate Change Initiative (CCI). We thank ESA/DLR for providing us with SCIAMACHY Level 1 data products and JAXA for GOSAT Level 1B data. We also thank ESA for making these GOSAT products available via the ESA Third Party Mission archive. We also thank the TCCON team (in particular P. Wennberg, CalTech) for providing TCCON data (obtained via <http://tccon.ornl.gov>), the European MACC/CAMS projects for providing CO<sub>2</sub> model fields (obtained from <http://macc.copernicus-atmosphere.eu/>) and NOAA/ESRL for providing CarbonTracker data (obtained via <http://www.esrl.noaa.gov/gmd/ccgg/carbontracker/>).

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