This manuscript version is made available under the CC-BY-NC-ND 4.0 license
<http://creativecommons.org/licenses/by-nc-nd/4.0/>

**The Greenhouse Gas Climate Change Initiative (GHG-CCI): comparison and quality
assessment of near-surface-sensitive satellite-derived CO₂ and CH₄ global data sets**

M. Buchwitz^{1,}, M. Reuter¹, O. Schneising¹, H. Boesch², S. Guerlet^{3, #}, B. Dils⁴, I. Aben³, R. Armante⁶, P. Bergamaschi¹⁰, T. Blumenstock⁷, H. Bovensmann¹, D. Brunner⁸, B. Buchmann⁸, J. P. Burrows¹, A. Butz⁷, A. Chédin⁶, F. Chevallier⁹, C. D. Crevoisier⁶, N. M. Deutscher^{1, 16}, C. Frankenberg^{11,20}, F. Hase⁷, O. P. Hasekamp³, J. Heymann¹, T. Kaminski¹², A. Laeng⁷, G. Lichtenberg⁵, M. De Mazière⁴, S. Noël¹, J. Notholt¹, J. Orphal⁷, C. Popp^{8, §}, R. Parker², M. Scholze^{12,13}, R. Sussmann⁷, G. P. Stiller⁷, T. Warneke¹, C. Zehner¹⁴, A. Bril¹⁵, D. Crisp¹¹, D. W. T. Griffith¹⁶, A. Kuze¹⁷, C. O'Dell¹⁸, S. Oshchepkov¹⁵, V. Sherlock¹⁹, H. Suto¹⁷, P. Wennberg²⁰, D. Wunch²⁰, T. Yokota¹⁵, Y. Yoshida¹⁵*

- 1. Institute of Environmental Physics (IUP), University of Bremen, Bremen, Germany*
- 2. University of Leicester, Leicester, United Kingdom.*
- 3. SRON Netherlands Institute for Space Research, Utrecht, Netherlands.*
- 4. Belgian Institute for Space Aeronomy (BIRA), Brussels, Belgium.*
- 5. Deutsches Zentrum für Luft- und Raumfahrt (DLR), Oberpfaffenhofen, Germany.*
- 6. Laboratoire de Météorologie Dynamique (LMD), Palaiseau, France.*
- 7. Karlsruhe Institute of Technology (KIT), Karlsruhe and Garmisch-Partenkirchen, Germany.*
- 8. Swiss Federal Laboratories for Materials Science and Technology (Empa), Dübendorf, Switzerland.*
- 9. Laboratoire des Sciences du Climate et de l'Environnement (LSCE), Gif-sur-Yvette, France.*
- 10. European Commission Joint Research Centre (EC-JRC), Institute for Environment and Sustainability (IES), Air and Climate Unit, Ispra, Italy.*
- 11. Jet Propulsion Laboratory (JPL), Pasadena, California, United States of America.*
- 12. FastOpt GmbH, Hamburg, Germany.*
- 13. University of Bristol, Bristol, United Kingdom.*
- 14. European Space Agency (ESA), ESRI, Frascati, Italy.*
- 15. National Institute for Environmental Studies (NIES), Tsukuba, Japan.*
- 16. University of Wollongong, Wollongong, Australia.*
- 17. Japan Aerospace Exploration Agency (JAXA), Tsukuba, Japan.*
- 18. Colorado State University (CSU), Fort Collins, Colorado, United States of America.*

19. National Institute of Water and Atmospheric Research (NIWA), Lauder, New Zealand.

20. California Institute of Technology, Pasadena, California, United States of America.

#) Now at: Laboratoire de Météorologie Dynamique (LMD), Institut Pierre-Simon Laplace, Paris, France.

§) Now at: National Museum of Natural History, Smithsonian Institution, Washington, DC, USA, and Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts, USA.

*) Corresponding author: Michael Buchwitz, Institute of Environmental Physics (IUP), University of Bremen, FB1, Otto Hahn Allee 1, 28334 Bremen, Germany, Phone: +49-(0)421-218-62086, Fax: +49-(0)421-218-62070, E-mail: Michael.Buchwitz@iup.physik.uni-bremen.de.

Abstract

The GHG-CCI project is one of several projects of the European Space Agency's (ESA) Climate Change Initiative (CCI). The goal of the CCI is to generate and deliver data sets of various satellite-derived Essential Climate Variables (ECVs) in line with GCOS (Global Climate Observing System) requirements. The "ECV Greenhouse Gases" (ECV GHG) is the global distribution of important climate relevant gases – atmospheric CO₂ and CH₄ - with a quality sufficient to obtain information on regional CO₂ and CH₄ sources and sinks. Two satellite instruments deliver the main input data for GHG-CCI: SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT. The first order priority goal of GHG-CCI is the further development of retrieval algorithms for near-surface-sensitive column-averaged dry air mole fractions of CO₂ and CH₄, denoted XCO₂ and XCH₄, to meet the demanding user requirements. GHG-CCI focusses on four core data products: XCO₂ from SCIAMACHY and TANSO and XCH₄ from the same two sensors. For each of the four core data products at least two candidate retrieval algorithms have been independently further developed and the corresponding data products have been quality-assessed and inter-compared. This activity is referred to as "Round Robin" (RR) activity within the CCI. The main goal of the RR was to identify for each of the four core products which algorithms should be used to generate the Climate Research Data Package (CRDP). The CRDP will essentially be the first version of the ECV GHG. This manuscript gives an overview of the GHG-CCI RR and related activities. This comprises the establishment of the user requirements, the improvement of the candidate retrieval algorithms and comparisons with ground-based observations and models. The manuscript summarizes the final RR algorithm selection decision and its justification. Comparison with ground-based Total Carbon Column

Observing Network (TCCON) data indicates that the “breakthrough” single measurement precision requirement has been met for SCIAMACHY and TANSO XCO₂ (< 3 ppm) and TANSO XCH₄ (< 17 ppb). The achieved relative accuracy for XCH₄ is 3-15 ppb for SCIAMACHY and 2-8 ppb for TANSO depending on algorithm and time period. Meeting the 0.5 ppm systematic error requirement for XCO₂ remains a challenge: approximately 1 ppm has been achieved at the validation sites but also larger differences have been found in regions remote from TCCON. More research is needed to identify the causes for the observed differences. In this context GHG-CCI suggests taking advantage of the ensemble of existing data products, for example, via the EnSeMble Median Algorithm (EMMA).

Keywords: SCIAMACHY, GOSAT, Greenhouse gases, Carbon dioxide, Methane, Climate Change

1. Introduction

Carbon dioxide (CO₂) is the most important anthropogenic greenhouse gas (GHG) contributing to global warming (Solomon et al., 2007). Despite its importance, our knowledge of the CO₂ sources and sinks has significant gaps (e.g., Stephens et al., 2007, Canadell et al., 2010) and despite efforts to reduce CO₂ emissions, atmospheric CO₂ continues to increase at a rate of approximately 2 ppm/year (Figure 1 top panel; see also Schneising et al., 2011, and references given therein; for a detailed discussion of Fig. 1 see Sect. 4). An improved understanding of the CO₂ sources and sinks is needed for reliable prediction of the future climate of our planet (Solomon et al., 2007). This is also true for methane (CH₄, Figure 1 bottom panel). Atmospheric methane levels increased until about the year 2000, were rather stable during ~2000-2006, but started to increase again in recent years (Rigby et al., 2008, Dlugokencky et al., 2009, Schneising et al., 2011, Frankenberg et al., 2011). Unfortunately, it is not well understood why methane was stable in the years before 2007 (e.g., Simpson et al., 2012) nor why it started to increase again at a rate of approximately 7-8 ppb/year (Schneising et al., 2011). Global satellite observations sensitive to near-surface CO₂ and CH₄ variations can contribute to a better understanding of the regional sources and sinks of these important greenhouse gases. Information on GHG surface fluxes (emissions and uptake) can be obtained by inverse modeling of

surface fluxes (e.g., Chevallier et al., 2007, Bergamaschi et al., 2009), where satellite observations are compared with predictions of a (chemistry) transport model (e.g., Figure 2) and satellite minus model mismatches are minimized by modifying the surface fluxes used by the model. This requires satellite retrievals to meet challenging requirements, as small errors of the satellite-retrieved atmospheric GHG distributions may result in large errors of the inferred GHG surface fluxes (e.g., Meirink et al., 2006, Chevallier et al., 2005). Instead of direct optimization of surface fluxes it is also possible to optimize (other) model parameters used to model the fluxes, as done in Carbon Cycle Data Assimilation Systems (CCDAS) (e.g., Kaminski et al., 2010, 2012) or other approaches (e.g., Bloom et al., 2010).

The goal of the GHG-CCI project is to generate the Essential Climate Variable (ECV) Greenhouse Gases (GHG) as defined by GCOS (Global Climate Observing System): “Distribution of greenhouse gases, such as CO₂ and CH₄, of sufficient quality to estimate regional sources and sinks” (GCOS, 2006). In order to get information on regional GHG sources and sinks, satellite measurements must be sensitive to near-surface GHG concentration variations. Currently only two satellite instruments deliver (or have delivered until recently) measurements which fulfill this requirement: SCIAMACHY on ENVISAT (March 2002 – April 2012) (Bovensmann et al., 1999) and TANSO-FTS on-board GOSAT (launched in January 2009) (Kuze et al., 2009). Both instruments perform (or have performed) nadir observations of reflected solar radiation in the near-infrared/short-wave-infrared (NIR/SWIR) spectral region, covering the relevant absorption bands of CO₂ and CH₄. They also cover the O₂ A-band spectral region to obtain “dry-air columns” needed for computing GHG dry-air column averaged mole fractions and/or to obtain information on clouds and aerosols. These two instruments are therefore the two core sensors used by GHG-CCI and the near-surface-sensitive column-averaged dry air mole fractions of atmospheric CO₂ and CH₄, denoted XCO₂ (in ppm) and XCH₄ (in ppb), are the core data products of GHG CCI. In addition, other sensors or viewing modes are also used (e.g., MIPAS/ENVISAT and SCIAMACHY solar occultation mode for stratospheric CH₄ profiles and IASI/METOP for mid/upper tropospheric CO₂ and CH₄ columns) as they provide additional constraints for atmospheric layers above the planetary boundary layer. The focus of the first two years

of the GHG-CCI project (September 2010 – August 2012) was to develop existing retrieval algorithms further, in order to improve the accuracy of the retrieved GHG data products.

The focus of GHG-CCI lies on ECV Core Algorithms (ECAs) and their core data products XCO₂ and XCH₄, which is also the focus of this manuscript. Other algorithms, referred to as Additional Constraints Algorithms (ACAs), are algorithms to retrieve CO₂ and/or CH₄ information from satellite data which have no or only little near surface sensitivity but are sensitive to GHG variations in upper layers (the ACAs are listed in Table 3 and further discussed in Section 6).

Several existing candidate ECAs were selected at the outset of the project for ongoing development, and have been iteratively improved upon through the course of the algorithm inter-comparison and validation activity. This activity is referred to as “Round Robin” (RR) exercise within the CCI.

The goal of the RR was to determine which ECA performs best to generate a given GHG-CCI core data product. The selected ECAs will be used in the third year of this project to generate the Climate Research Data Package (CRDP), which will essentially be the first version of the ECV GHG. The description of the RR approach and its results is the focus of this manuscript. Note that previous publications focused on individual algorithms and their data product. Only recently have results obtained using different algorithms been compared, most notably by Oshchepkov et al., 2012, for TANSO/GOSAT XCO₂. This manuscript is therefore one of the first focusing on inter-comparisons.

This manuscript is structured as follows: Section 2 presents an overview of the GHG-CCI project followed by a description of the user requirements in Section 3. In Section 4 the retrieval algorithms are briefly described. The main part of this manuscript is Section 5 where the RR approach and its main results are presented and discussed. Section 6 provides a short overview of the Additional Constraints Algorithms (ACAs) also used within GHG-CCI but not the focus of this manuscript. Section 7 gives a short overview of the Climate Research Data Package (CRDP) to be generated using the selected algorithms. A summary and conclusions are given in Section 8.

2. GHG-CCI project overview

The GHG-CCI project covers all aspects needed to generate the ECV GHG and to assess its quality and usefulness. This includes the use of appropriate satellite instruments (primarily SCIAMACHY/ENVISAT and TANSO/GOSAT to generate global XCO₂ and XCH₄ time series), calibration aspects (related to "Level 0-1 processing", primarily for SCIAMACHY), and development and application of retrieval algorithms to convert the satellite-measured spectra into atmospheric CO₂ and CH₄ information ("Level 1-2 processing"). Also included is the analysis of the resulting global data sets, including validation and user assessments, focusing on inverse modeling of regional surface fluxes (i.e., "Level 2-4 processing"). Note that the fluxes (Level 4 products) will most likely be derived from Level 2 data rather than from (spatio-temporally averaged and potentially gap-filled) Level 3 data products, as Level 2 data contain more information than those at Level 3 and usually benefit from better error characterization.

Level 1 data (i.e., geolocated and calibrated radiances) are input data for CCI (i.e., Level 0-1 processing is covered by other projects). SCIAMACHY Level 0-1 processing experts are part of the GHG-CCI team in order to provide expertise and to ensure that the findings of the study feed back to improve future Level 1 data products if necessary. Close links have been established with the GOSAT team at JAXA for GOSAT Level 1 data access, expertise and feedback.

The SCIAMACHY and TANSO Level 1 data products are de-facto used as Fundamental Climate Data Records (FCDRs, see GCOS, 2006) despite the fact that no dedicated inter-calibration or merging efforts are currently foreseen. Consistency between the time series of the two GHG-CCI core satellites is addressed at the level of the Level 2 data products. Ideally, an ECV data product or Thematic Climate Data Record (TCDR) of a given quantity should be a single merged data record obtained from all available appropriate sensors such as SCIAMACHY and TANSO for satellite-derived XCO₂. However, within the present initial stage of this project only first steps in this direction have been carried out (see Section 5).

The ground-based validation of the "satellite-derived" XCO₂ and XCH₄ data products largely relies on the Total Carbon Column Observing Network (TCCON) (Wunch et al., 2010, 2011a) as this network

has been designed and developed for this purpose. Methods to also use data from other sources in the future (e.g., NDACC (see Susstmann et al., 2013), GAW) are being developed in parallel. Aircraft observations, e.g., HIPPO (e.g., Wofsy, 2011, Wecht et al., 2012), are also interesting, but have not yet been used directly (indirectly some of these data have been used via the calibration of TCCON, see Sect. 5.2.1).

A dedicated GHG-CCI Climate Research Group (CRG) has been set up to represent the users of the satellite-derived CO₂ and CH₄ data products and to provide expertise on inverse modeling of surface fluxes, CCDAS and other user related aspects. A strong link exists between GHG-CCI and the EU FP7 GMES project MACC-II (Monitoring of Atmospheric Composition and Climate - Interim Implementation, <http://www.gmes-atmosphere.eu/>) that provides feedback on the data quality.

Key activities carried out in the first two years of this project were the establishment of the user requirements (Section 3), the further development of retrieval algorithms (described briefly in Section 4) and data processing and data analysis with the goal of identifying which algorithms perform best (“Round Robin” (RR)). The description of these RR activities and their results is the focus of this manuscript (Section 5). In the third year of this project the selected algorithms will be used to generate the CRDP (see Section 7), which will subsequently be validated and assessed by users.

3. User requirements

An important initial activity carried out in this project was the establishment of the user requirements. They have been formulated in detail in the GHG-CCI User Requirements Document (URD) (Buchwitz et al., 2011a). The requirements are based on peer-reviewed publications primarily prepared in the context of existing or planned satellite missions and GHG-CCI CRG user expertise and experience with existing satellite data.

Most critical are the requirements on random and systematic errors listed in Table 1. The most challenging requirement is the one on biases for XCO₂. The threshold requirement is 0.5 ppm because even errors of a few tenths of a ppm can result in large errors of the inferred CO₂ surface fluxes when used as input data for inverse modeling schemes (e.g., Chevallier et al., 2005). However, to what

extent systematic errors result in biases of the inferred fluxes depends on the spatio-temporal pattern of the systematic errors. A global bias, even if considerably larger than the required 0.5 ppm, would not be critical because it can easily be detected and corrected *ad hoc*. Most critical are state-dependent systematic errors, which result in regional-scale (~1000 km) biases on medium time scales (~monthly), because they will likely be missed by bias-correction schemes. As the overall impact of the atmospheric concentration error on the surface flux error depends on the spatio-temporal pattern of the concentration error, the values listed in Table 1 have to be interpreted with care. The requirements reflect what the GHG-CCI users would like to see achieved. The utility of the data can ultimately only be determined by careful analysis. The numbers listed in Table 1 serve to give a rough indication of the required uncertainties but should not be over-interpreted.

The requirements for XCH₄ are also challenging but somewhat less demanding than those for XCO₂. The main reason is that XCH₄ is more variable compared to XCO₂ relative to its background value on the spatio-temporal scales relevant for the satellite retrievals (e.g., Frankenberg et al., 2005, 2011, Meirink et al., 2006, Bergamaschi et al., 2009, Schneising et al., 2011, 2012).

4. Retrieval algorithms

In this section, a brief overview of each retrieval algorithm used for the GHG-CCI RR is given. The reader is referred to peer-reviewed publications for details. All algorithms used within the GHG-CCI RR are also described in the GHG-CCI Algorithm Theoretical Basis Document (ATBD) (Reuter et al., 2012a).

The ECV Core Algorithms (ECAs) generate one or more of the four GHG-CCI core data products, XCO₂ (in ppm) and XCH₄ (in ppb) from SCIAMACHY and TANSO (each of the four combinations is a separate product). An overview of these algorithms is given in Table 2 and briefly described in the following sub-sections. Results obtained with all ECAs are shown in Fig. 1: the top panel shows northern hemispheric (NH) time series of XCO₂ and the bottom panel XCH₄ time series. As can be seen, the various XCO₂ time series (generated with the various algorithms described in the following sub-sections) are similar but not exactly identical. There are clear differences, e.g., a difference of the seasonal cycle amplitude, between the two SCIAMACHY algorithms WFMD (Schneising et al., 2011,

Heymann et al., 2012b) and BESD (Reuter et al., 2011) likely due to sub-visual cirrus clouds not explicitly considered by WFMD. Differences are also due to the different spatial sampling of the various data products. From Figure 1 it can therefore typically not be concluded which data product is the most accurate. This requires, for example, a careful comparison with independent accurate ground-based observations (see Section 5.2). However, one obvious problem can be identified: the SCIAMACHY XCH₄ product generated with the IMAP algorithm (Frankenberg et al., 2011) suffers from a significant high bias (relative to several other TANSO/GOSAT XCH₄ data products) during the year 2010 (highlighted by the dotted line). This problem is related to SCIAMACHY detector degradation issues which are not yet properly dealt with by the SCIAMACHY radiometric calibration nor compensated by the IMAP algorithm (note that the second SCIAMACHY XCH₄ algorithm WFMD (Schneising et al., 2011) has not yet been applied to 2010 data; the WFMD time series covers only the years 2003-2009). As will be discussed in more detail below, the most challenging problems addressed within GHG-CCI are related to achieving the required accuracy: for XCO₂ this is a challenge because of demanding user requirements and for XCH₄ the most important challenge was to deal with the progressive SCIAMACHY detector degradation in the spectral region needed for methane retrieval which started in October 2005 (see Schneising et al., 2011, and Frankenberg et al., 2011, for a detailed discussion).

4.1 Full Physics (FP) and Proxy (PR) algorithms

Within GHG-CCI, two types of ECAs can be distinguished: The “Full Physics” (FP) algorithms and the light path “Proxy” (PR) algorithms (see also Schepers et al., 2012).

FP algorithms model all relevant physical effects such as scattering by aerosols and clouds and have corresponding elements as part of the state vector, which contains all parameters which are to be retrieved. The FP algorithms obtain the dry air column-averaged mole fraction (needed to compute the dry air column-averaged mole fractions of the GHG, i.e., XCO₂ and/or XCH₄) either from the retrieved surface pressure or using meteorological information.

The PR algorithms are based on computing the dry air column-averaged mole fraction using a “reference gas”, which has to be much less variable than the gas of interest on the relevant spatio-temporal scales. The PR method is used for XCH₄ retrieval using CO₂ as a reference gas. The XCH₄ is essentially obtained from computing the ratio of the retrieved CH₄ column and the retrieved CO₂ column. The advantage of this method is that it is potentially very fast, accurate and robust (as several systematic errors cancel in the CH₄/CO₂ column ratio). The disadvantage is that a correction is needed for CO₂ variability, typically based on a global model (see, e.g., Frankenberg et al., 2005, 2011, Parker et al., 2011, Schneising et al., 2009, 2011, Schepers et al., 2012).

4.2 SCIAMACHY XCO₂ algorithms

The Weighting Function Modified (WFM) Differential Optical Absorption Spectroscopy (DOAS) algorithm (WFM-DOAS or WFMD) has been developed to retrieve vertical columns of several atmospheric gases including the GHGs discussed in this manuscript (Buchwitz et al., 2000). During the last decade, this algorithm has been significantly improved and used to generate global multi-year XCO₂ and XCH₄ data sets from SCIAMACHY (Buchwitz et al., 2005, 2007; Schneising et al., 2008, 2009). Within GHG-CCI, WFMD has been further improved and used to generate long-term consistent time series (Schneising et al., 2011, 2012, Heymann et al., 2012a, 2012b). WFMD has been implemented as a fast look-up table (LUT) based retrieval scheme to avoid time consuming radiative transfer (RT) simulations. WFMD is a least-squares method using a single constant atmospheric prior (e.g., single constant CO₂ and CH₄ mixing ratio profiles, a single aerosol scenario, no clouds). WFMD can process one orbit of SCIAMACHY observations in a few minutes on a single workstation. Aerosols and cirrus clouds are only treated approximately by considering spectrally broad band effects by a low-order polynomial and by post-processing filtering. Overall, this results in small but significant biases, especially for XCO₂ (Heymann et al., 2012a). Recently, an improved version of WFMD has been developed for SCIAMACHY XCO₂ retrieval (Heymann et al., 2012b, see also Figure 2) and the XCO₂ data set generated with this latest version has been used for the GHG-CCI RR. For SCIAMACHY XCH₄ retrieval, the WFMD version described in Schneising et al., 2011, 2012, has been used (see below).

The Bremen Optimal Estimation DOAS (BESD) FP algorithm was specifically developed for accurate and precise SCIAMACHY XCO₂ retrieval considering aerosols and clouds thereby overcoming limitations of the WFMD algorithm (Reuter et al., 2010, 2011). In contrast to WFMD, BESD is not based on a LUT scheme but uses on-line RT model simulations. BESD is therefore computationally much more demanding. Also, unlike WFMD, BESD is based on Optimal Estimation (OE, Rodgers, 2000) and aerosol and cirrus parameters are state vector elements and retrieved in addition to XCO₂.

4.3 TANSO XCO₂ algorithms

Both GHG-CCI TANSO XCO₂ retrieval algorithms are FP algorithms: the University of Leicester's (UoL) OCO (Orbiting Carbon Observatory, Crisp et al., 2004) FP ("UoL-FP" or OCFP) algorithm (Cogan et al., 2012, Parker et al., 2011) and the RemoteC (or SRON Full Physics (SRFP)) algorithm (Butz et al., 2011). Both algorithms are based on adjusting parameters of a surface-atmosphere state vector and other parameters to the satellite observations, but differ in many details (different RT models, different inversion schemes (OE or Tikhonov-Phillips), different schemes for aerosol modeling and inversion, use of different pre-processing and post-processing steps, etc.) as discussed in Cogan et al., 2012, Parker et al., 2011, and Butz et al., 2011.

4.4 SCIAMACHY XCH₄ algorithms

For SCIAMACHY XCH₄ retrievals, PR algorithms are used: WFMD (Schneising et al., 2011, see above) and IMAP (Iterative Maximum A Posteriori) DOAS (Frankenberg et al., 2011). These algorithms were already well developed when GHG-CCI started but had essentially only been applied to retrieve XCH₄ from the first three years of the ENVISAT mission (e.g., Schneising et al., 2008). Within GHG-CCI, this time series has been significantly extended. The key challenge was (and partly still is, see Figure 1) to deal with the significant detector degradation in the spectral region needed for methane retrievals after 2005 (see Frankenberg et al., 2011, and Schneising et al., 2011, for details).

4.5 TANSO XCH₄ algorithms

To overcome the key limitation of the XCH₄ PR algorithms, namely the need to correct the retrieved XCH₄ for CO₂ variations using a model, FP algorithms are also used within GHG-CCI, but only for TANSO. TANSO has higher spectral resolution than SCIAMACHY which is exploited to also retrieve scattering parameters in addition to CH₄. Two TANSO XCH₄ FP retrieval algorithms are being used within GHG-CCI, which are also used for TANSO XCO₂ retrieval (see above), OCFP (Parker et al., 2011) and SRFP (Butz et al., 2011), in addition to the two PR algorithms OCPR (Parker et al., 2011) and SRPR (Schepers et al., 2012).

5. Round Robin approach and results

In this section an overview of the GHG-CCI Round Robin (RR) activities is given which have been carried out in the first two years of this project.

5.1 Round Robin approach

The ultimate goal of the GHG-CCI RR was to identify which algorithms and corresponding data products to use for generating the CRDP. This comprised the further development of existing retrieval algorithms with the goal of meeting the challenging user requirements, the application of these algorithms to generate global multi-year XCO₂ and XCH₄ sets, the comparison with ground-based reference data and inter-comparisons of the data products generated with the competing ECAs.

The selection procedure for ECAs and ACAs is described in the GHG-CCI Round Robin Evaluation Protocol (RREP, Buchwitz et al., 2011b). Initially the plan was to develop a score-based selection scheme, i.e., to compute a single number for each algorithm / data product (the higher the number, the better the algorithm), mainly based on satellite – ground-based observation differences. However, this was not pursued because a scientifically sound basis for the classification could not be established. Instead a set of Figures of Merit (FoM), mostly based on differences between satellite and ground-based observations, have been defined (see RREP, Buchwitz et al., 2011b) and evaluated. However, as explained in the RREP and also shown in this manuscript, the comparison with the ground-based observations is only one component for the final selection primarily because of the sparseness of the

ground-based network (see Section 5.2). Another major component of the selection procedure was the analysis of (global and regional) maps and time series, including comparisons with global state-of-the-art models, and inter-comparisons of the data products generated with the different candidate algorithms. Note that “blind testing” has not been used as it would have been possible to identify the algorithms/products by using some of their characteristics such as averaging kernels and spatial coverage. Some key results of this RR activity are presented here including a summary of the main RR decision results given in Section 5.6 for ECAs and Section 6 for ACAs.

According to the initial ESA specification of the CCI RR exercise it was required to evaluate “algorithms”. However, complex algorithms such as the ones used within GHG-CCI can hardly be evaluated, especially not in terms of identifying “the best one” in terms of smallest biases when applied to real data. Simulated retrievals have been performed (see, e.g., Buchwitz et al., 2011c, 2012a, and references given therein) but only for the individual algorithms and not in a consistent manner. This would have been a major activity incompatible with the CCI schedule especially if the goal would have been to obtain a better understanding of the differences between the data products obtained from the real observations. In this context it has not been identified that any of the algorithms suffer from obvious shortcomings. All XCO₂ algorithms, for example, use different approaches to mitigate biases due to scattering by aerosols and (thin) clouds, but it is virtually impossible to identify *a priori*, e.g., based on a description of the algorithms and the simulation results, which of the approaches will result in the smallest XCO₂ or XCH₄ biases when applied to real data.

What has been evaluated in detail are the end products, i.e., the quality of the XCO₂ and XCH₄ data products. This means that primarily data products have been evaluated during RR but not algorithms. As shown in this manuscript, this is not a trivial task, e.g., due to the sparseness of the TCCON reference data. Therefore, as shown in this manuscript, the RR decisions are not only based on comparisons with TCCON. The satellite retrieval team focused on producing the best possible end products. Which input data to use and how to treat them, e.g., in a dedicated pre-processing step, has not been prescribed. Pre-processing steps may be critical for the quality of the end product. This is particularly true if the instrument shows significant degradation as is the case for SCIAMACHY after

2005 especially in the spectral region needed for methane retrieval. To deal with this, quite different approaches have been used by the two algorithms IMAP (Frankenberg et al., 2011) and WFMD (Schneising et al., 2011, 2012). For example, IMAP uses as input data spectra that have been specifically calibrated at SRON and IMAP also uses a single so-called “Dead and Bad detector Pixel Mask” (DBPM), needed to reject detector pixels which are not useful. In contrast, WFMD uses the official standard SCIAMACHY Level 1 data product with standard calibration and several DBPMs, each optimized for a certain time period, typically covering one or more years (see Schneising et al., 2011, for details).

Finally, it is important to highlight the preliminary nature of the RR. This is due to the fact that all Level 1 input data and retrieval algorithms are continuously being improved. An algorithm / data product currently identified to be the best one will not necessarily be the best one in the future. GHG-CCI therefore needs to be flexible and will aim to consider this in future phases of the CCI.

5.2 Comparison with ground-based (TCCON) observations

5.2.1 TCCON data and error characteristics

The most relevant ground-based observations for the validation of the satellite-derived XCO₂ and XCH₄ data products are the corresponding data products of the TCCON. The TCCON data products have been obtained from the TCCON website (www.tcon.caltech.edu/; latest access Feb. 2012 using version GGG2009, i.e., not the latest version GGG2012, which was not available for the GHG-CCI Round Robin comparison) or have been provided by the TCCON PIs. The TCCON products have been calibrated to WMO/GAW in situ trace gas measurement scales using aircraft observations (Wunch et al., 2010, Deutscher et al., 2010, Geibel et al., 2012, Messerschmidt et al., 2012). The best independent estimates of the TCCON inter-site comparability to date are provided by these independent aircraft calibration data. While not exhaustive, these demonstrate consistency at the 0.1% level (1-sigma) for XCO₂ (~0.4 ppm) and 0.2% for XCH₄ (~4 ppb), with no obvious inter-hemispheric differences (Wunch et al., 2010). Nevertheless, the TCCON team recognizes that inter-site comparability needs to be better characterized, especially for methane (e.g., at Darwin and Wollongong, not discussed in the references cited above), and work is in progress to achieve this. The

systematic and random errors of single TCCON data are therefore typically 0.4 ppm for XCO₂ (1-sigma) and 4 ppb (1-sigma) for XCH₄ (Notholt et al., 2012, based on Wunch et al., 2010). Due to these 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, i.e., the satellite data errors are likely smaller than reported here.

5.2.2 Inter-comparison method

Different inter-comparison methods have been used, e.g., to ensure robustness of the findings. In addition to the method used and results obtained by the validation team (Notholt et al., 2012), which are summarized in this manuscript, independent inter-comparisons of the satellite data products with TCCON have also been carried out by the satellite data product provider (Buchwitz et al., 2012a). The methods differ by various aspects such as investigated time period and direct comparison or comparison after transformation to common *a priori* profiles and application of averaging kernels. Each satellite data product provider performed an independent validation of his data product (considering averaging kernels or not) covering the entire time series (to the extent possible given the limitations of the TCCON data, see Tab. 4). In contrast, the validation team has applied the same method to all satellite data products and has, for a given product, only used a time period where data from all competing algorithms were available (SCIAMACHY: XCO₂: 2006-2009; XCH₄: 2003-2009, TANSO: mid 2009-2010).

The method used by the validation team is based on a direct comparison of the co-located satellite and TCCON data products. No correction for different *a priori* profiles and averaging kernels has been applied. Note that it is not trivial to consider averaging kernels for the XCO₂ and XCH₄ satellite and TCCON retrievals as strictly speaking this requires a reliable estimate of the real atmospheric variability, which is unknown. This aspect is discussed in detail in Wunch et al., 2011b, where the impact of this correction for TANSO XCO₂ is discussed at Lamont, USA, where the real variability of the CO₂ profiles is obtained using regular aircraft and other observations. For the global data sets this is not possible. Nevertheless, for some of the satellite products, averaging kernels have been applied by the satellite data provider. For example, Reuter et al., 2013, has applied individual averaging

kernels for all XCO₂ products from SCIAMACHY and TANSO by adjusting all retrievals to a
 common *a priori* using the Simple Empirical CO₂ Model (SECM) described in Reuter et al., 2012b.
 They found that the adjustments are typically a few tenth of a ppm. Reuter et al., 2012b, estimated the
 smoothing errors and found that it is typically 0.17 ppm for SCIAMACHY XCO₂ and 0.05 ppm for
 TCCON XCO₂. These results indicate that the impact of applying or not applying the averaging
 kernels for satellite – TCCON comparisons is small. The reason is that the averaging kernels of the
 TCCON and the satellite data are close to unity and the resulting smoothing error is therefore typically
 quite small, especially for XCO₂. For methane the (relative) smoothing errors are somewhat larger, as
 methane is more variable. For example, Parker et al., 2011, found that “the mean smoothing error
 difference included in the GOSAT to TCCON comparisons can account for 15.7 to 17.4 ppb for the
 northerly sites and for 1.1 ppb at the lowest latitude site”. For the SCIAMACHY XCH₄ validation
 results presented in Schneising et al., 2012, it has been found that applying averaging kernels (by
 using TM5 model profiles as a common *a priori*) leads to adjustments of 0.4% (approx. 7 ppb).
 Overall it has been found that the validation results obtained by the validation team (Notholt et al.,
 2012) and the satellite data provider (Buchwitz et al., 2012a), where averaging kernels have been
 applied for at least some of the products, agree well, especially for XCO₂ (Buchwitz et al., 2012b).
 The comparison of the various methods used to quantify random and systematic errors of the satellite
 products (Buchwitz et al., 2012b) indicates that the RR validation results are robust.

In the following, the results obtained by the validation team are presented. Detailed results will be
 reported elsewhere (Dils et al., manuscript in preparation, preliminary title: “The Greenhouse Gas
 Climate Change Initiative (GHG-CCI): Comparative validation of SCIAMACHY and TANSO-FTS
 CO₂ and CH₄ retrieval algorithm products with measurements from the TCCON network”). Therefore
 we here give only a short overview highlighting major findings.

For each product and each TCCON site a number of Figures of Merit (FoMs) have been computed by
 the validation team. Key results are shown in Fig. 3 for XCO₂ and Fig. 4 for XCH₄, discussed in detail
 in dedicated sub-sections below. Shown are comparisons of the four GHG-CCI core data products
 generated with two or more of the candidate algorithms at the 10 TCCON sites listed in Table 4. The

results shown in Figs. 3 and 4 have been generated using a spatio-temporal co-location criterion of 2 hours and 500 km (for alternative co-location criteria see Notholt et al., 2012). Several numerical values are given, which are also listed in Table 5, computed from satellite minus TCCON differences for each single satellite retrieval and the corresponding TCCON mean value. On the left hand side of Figs. 3 and 4 the mean satellite-TCCON differences are shown for each of the 10 TCCON sites and all four core data products and their corresponding ECAs. For each ECA the standard deviation of the station-to-station bias has been computed (“StdDev”) and the total number of co-located satellite retrievals used for comparison (“N”). The standard deviation of the station-to-station bias is interpreted as a relevant measure of the systematic error (“relative accuracy” or “relative bias”). The standard deviation is more relevant to characterize systematic errors compared to, for example, the mean difference. Most critical is to achieve high “relative accuracy” (or low “relative bias”) not necessarily high “absolute accuracy” (although this would of course be better). For example, a constant offset of the satellite data would not be critical if the data are being used for surface flux inverse modeling (see Section 3) and this is considered by computing the standard deviation. On the right hand side of Figs. 3 and 4 the standard deviations of the satellite-TCCON differences are shown for each TCCON site. They are a measure of the random error (scatter) of the satellite retrievals. The corresponding mean value over all TCCON sites is used to characterize the mean random error (or “precision”) of the corresponding satellite data product. In the following, Figs. 3 and 4 are discussed in more detail for each of the products.

5.2.3 Satellite XCO₂ comparisons with TCCON

The comparison of the two SCIAMACHY XCO₂ retrieval algorithms WFMD and BESD with TCCON shows the following (Figure 3, top half): BESD has typically lower systematic errors (0.7 ppm) compared to WFMD (1.3 ppm) and also a higher precision (2.3 ppm compared to 5.1 ppm). Ultimately it can be expected that the biases of BESD will be even lower as it has been identified (not shown) that the BESD RR data set suffers from problems related to the SCIAMACHY Level 1 data product used (version 7 consolidation level u, “L1v7u”). This data product was used because it was the latest version available when the final RR data set had to be generated and because it also covers the

time period after 2009. The previous Level 1 version 6 (L1v6), used by WFMD, does not suffer from these problems but is only available until the end of 2009, where the WFMD data set ends. It has been found that BESD retrievals for selected months using the improved new version L1v7w have much lower biases especially because the many outliers caused by the L1v7u spectra are not present any more (not shown). It is therefore necessary and planned to reprocess the entire SCIAMACHY data set with BESD using L1v7w, e.g., for the generation of the CRDP. A potentially important pro for WFMD for certain applications is the much larger number of data points.

The comparison of the two TANSO XCO₂ retrieval algorithms OCFP and SRFP with TCCON shows the following (Figure 3, bottom half): The biases depend on site and are typically in the range +/- 1 ppm. They are very similar for both algorithms. This is also true for the standard deviation of the difference between the TANSO and TCCON estimates, which is typically in the range 2-3 ppm. The number of co-locations is also nearly identical for both algorithms but varies significantly from site to site, which is true for all comparisons shown in Figs. 3 and 4.

As shown in Table 5, the precision requirement for XCO₂ is met by all algorithms. WFMD meets the threshold requirement and the other algorithms including BESD even meet the breakthrough requirement. The challenging 0.5 ppm bias requirement has however not yet been met but several algorithms achieve a performance close to the threshold requirement (0.6-0.9 ppm, depending on algorithm).

5.2.4 Satellite XCH₄ comparisons with TCCON

The comparison of the two SCIAMACHY XCH₄ retrieval algorithms WFMD and IMAP with TCCON shows the following (Figure 4, top half): Overall, the systematic differences with respect to TCCON vary from site to site from nearly 0 ppb at Lamont to 20-30 ppb at the southern hemisphere (SH) sites Darwin, Wollongong, and Lauder, but are very similar for WFMD and IMAP. The reason for the large differences at these SH sites have not yet been identified. This is probably not due to the TCCON reference data as these differences are larger than the estimated TCCON inter-site comparability (see Sect. 5.2.1) and also the comparison with TANSO XCH₄ (see below) does not show this type of systematic deviation (the OCFP results however also show a low bias at the SH sites

compared to the northern sites esp. at Darwin). Agreement is within +/- 10 ppb if these SH sites are
 excluded. In order to obtain an estimate of the relative biases (i.e., considering that an overall offset is
 not critical), the standard deviation of the station-to-station biases has been computed: it amounts to 11
 ppb for WFMD and 15 ppb for IMAP. The standard deviation of the satellite-TCCON differences,
 which is a measure of the single measurement precision (1-sigma), is on average 82 ppb for WFMD
 and 50 ppb for IMAP. Because nearly all TCCON sites started operation after 2005 (see Table 4), i.e.,
 after the loss of important SCIAMACHY methane detector pixels due to detector degradation, the
 values listed for SCIAMACHY in Figure 4 are not representative for the years 2003-2005. Until the
 end of 2005 the performance was much better and the corresponding values are listed in curved
 brackets in Table 5. A possible explanation for the larger scatter (worse precision) of WFMD after
 2005 is that WFMD is an unconstrained least-squares algorithm whereas IMAP is based on Optimal
 Estimation and uses detailed CH₄ information (as a function of latitude, altitude and time but not
 longitude) from a global model as *a priori* information. This raises the question why the precision of
 the two data products is similar for 2003-2005. This could be related to the fact that only a single
 DBPM is used by IMAP whereas WFMD has used a DBPM optimized for 2003-2005. Another
 possible explanation could be the use of differently calibrated input data. As shown in Fig. 4, the
 number of satellite soundings used varies significantly from site to site, but overall is very similar for
 WFMD (N=37628) and IMAP (39489) (at least at TCCON sites, for other locations this may not be
 true, see Figures 9 and 10).

The comparison of the four TANSO XCH₄ retrieval algorithms (OCPR, OCFP, SRPR, SRFP) with
 TCCON shows the following (Figure 4, bottom half): The biases depend on the TCCON site but are in
 the range +/- 15 ppb. The estimated relative bias is best for OCPR (2 ppb) and worst for OCFP (8
 ppb). OCPR has the largest number of data points (followed by SRPR). The number of data points is
 higher for the PR algorithms (OCPR and SRPR) compared to the FP algorithms (OCFP and SRFP).
 The FP algorithm with the lowest relative bias is SRFP (3 ppb). The PR algorithm with the lowest
 relative bias is OCPR (2 ppb). The standard deviation of the satellite – TCCON differences are nearly
 identical for all four algorithms.

As shown in Table 5, the SCIAMACHY XCH₄ product for 2003-2005 meets the threshold precision requirement (but not for 2006 and later years due to the detector degradation). In contrast, the TANSO XCH₄ has a much higher precision and even the breakthrough precision requirement is met by all algorithms. All TANSO XCH₄ algorithms meet the relative accuracy (relative bias) user requirement - some are close to or even better than the goal requirement. For SCIAMACHY this is only true for 2003-2005.

Concerning the final RR algorithm selection decision, it is important not to over-interpret the numerical values listed in Table 5 due to the sparseness of the TCCON sites. For this and other reasons, the TCCON comparisons presented and discussed in this section are only one key component of the GHG-CCI RR activities. Therefore, more comparisons have been conducted, for XCO₂ and XCH₄, as described in the following.

5.3 Inter-comparison of XCO₂ data products

Within GHG-CCI two algorithms have been further developed to retrieve XCO₂ from SCIAMACHY, namely WFMD and BESD, and two algorithms to retrieve XCO₂ from TANSO, namely OCFP and SRFP. In addition, there are three non-European TANSO algorithms presented and discussed in the peer-reviewed literature whose data products have also been used for comparison: (i) the official operational TANSO algorithm (v02.xx) developed at the National Institute for Environmental Studies (NIES) in Japan (Yoshida et al., 2011; in the following referred to as “NIES” algorithm), (ii) a scientific algorithm called PPDF (Pathlength Probability Density Function) also developed at NIES (Bril et al., 2007, Oshchepkov et al., 2008, 2009, 2011, 2012), and (iii) NASA/JPL’s ACOS (Atmospheric CO₂ Observations from Space) v2.9 algorithm (O’Dell et al., 2012, Crisp et al., 2012).

The global XCO₂ data products from all 7 algorithms have been inter-compared within GHG-CCI (Reuter et al. 2013, Buchwitz et al., 2012a). The analysis revealed the following: The various satellite XCO₂ data products all capture the expected large scale variations of atmospheric CO₂ such as the time dependent north-south gradient (Figures 5 and 6, discussed below) and the CO₂ increase and seasonal cycle (Figure 1) but exhibit differences in the spatio-temporal pattern which – depending on region and time – may exceed the relative bias user requirement of 0.5 ppm.

Typical examples are shown in Figures 5 and 6. Figure 5 shows comparisons of the four GHG-CCI XCO₂ algorithms (BESD, WFMD, SRFP, OCFP). Figure 6 shows the GHG-CCI algorithms as well as the three non-European algorithms mentioned above (ACOS (v2.9), PPDF (NIES PPDF-D), and NIES (v02.xx)) for the two months September 2009 and May 2010. Also shown is the ensemble data product generated with the Ensemble Median Algorithm (EMMA) algorithm, discussed below, TCCON XCO₂, and XCO₂ from NOAA's CO₂ assimilation system CarbonTracker (CT) (Peters et al., 2007). As can be seen, all satellite retrieval algorithms capture the north-south XCO₂ gradient, which is significantly different for the two months shown, in good to reasonable agreement with TCCON and CarbonTracker (Figure 6). As can also be seen, differences between the data products often exceed 0.5 ppm, particularly at locations remote from TCCON sites (e.g., Sahara, South America, Africa). As discussed in Section 5.2, it appears virtually impossible to use TCCON to determine which algorithm performs best, at least for TANSO. For SCIAMACHY it has been shown that BESD outperforms WFMD in terms of single measurement precision and bias not however in terms of number of observations, which is significantly higher for WFMD. It is also likely that a "best data product" for all conditions does not exist at present as each retrieval algorithm is expected to have its strengths and weaknesses. Therefore, which algorithm performs best may depend on the spatio-temporal interval of interest. Clearly, more research is needed to understand the differences between the various XCO₂ data sets shown in Figures 5 and 6. One approach to further assess the relative quality of the various satellite-derived global XCO₂ data sets is to compare them with their median. This approach is presented in the following section.

5.3.1 Comparison with ensemble median (EMMA)

In this section we aim at answering two related questions: (i) How to determine which data product is likely "the best", if the largest differences are at locations remote from validation sites? (ii) Which data product should be used for inverse modeling of surface fluxes if all products differ and if it is not clear which product would give the most reliable results? To answer these questions we use the median of the various XCO₂ products. The situation appears to be similar to that for climate modeling: it is not clear which "model" is the best and (remote from validation sites) there is no truth to compare with. A

promising approach to deal with this is to make use of the fact that several state-of-the-art algorithms and corresponding XCO₂ data products are available, i.e., an ensemble of data products, which can be exploited. This is the underlying idea of the Ensemble Median Algorithm (EMMA, Reuter et al., 2013). As described in more detail below and in Reuter et al., 2013, EMMA computes the median of an ensemble of individual XCO₂ data products, which can be used for comparison with the individual data products, e.g., to identify outliers. However, the EMMA XCO₂ product has also been generated to be useful as a stand-alone XCO₂ data product for inverse modeling and other applications.

The strength of using an ensemble of satellite data products was highlighted at the end of the first year of the GHG-CCI project (Buchwitz et al., 2011c), when biases (0.5%) between Bialystok TCCON XCO₂ and co-incident satellite data were identified in the majority of algorithms participating in the GHG-CCI. This bias occurred due to an empirical correction of known magnitude, to account for a laser-sampling bias in the FTS data before September 21, 2009, inadvertently being applied in the wrong direction. A bias in XCH₄ in the early part of the Bialystok time series that occurred due to missing fits in one of the CH₄ micro-windows was also brought to light by comparisons to the ensemble of satellite retrievals. The identification and quantification of these biases would most likely not have been possible with a single algorithm / data product, due to difficulty in proving that such relatively small differences are not due to possible retrieval algorithm issues.

A detailed description of EMMA is presented in Reuter et al., 2013. Therefore here only a short overview is given. The presented version of EMMA (v1.3a) uses the 7 individual satellite XCO₂ products shown in Figs. 6 and 7 and generates a Level 2 product (i.e., a product containing the XCO₂ of the individual satellite soundings including uncertainty estimate and other information such as averaging kernels) using the median in each 10°x10° monthly grid cell (“voxel”). In short, EMMA works as follows: For each voxel, the mean XCO₂ value is computed for each of the 7 individual data products. The median of the 7 mean values determines which of the individual satellite Level 2 data products is used for the EMMA data product for that voxel (if a certain voxel is not covered by all 7 data products, a smaller number of data products is used). Using the median has several advantages compared to, for example, using the mean value. A key aspect is that the median is robust with respect

to outliers. Using the median essentially removes outliers. This is of critical importance as each of the individual data products appears to suffer from outliers but where they appear and when is not known *a priori* and depends on the algorithm. Of at least equal importance is that the GHG-CCI users need a Level 2 data product (individual soundings) and not a Level 3 data product (e.g., gridded monthly averages). Furthermore, the use of an ensemble of data products possibly permits the generation of more reliable uncertainty estimates, obtained from a combination of the ensemble scatter and the reported uncertainties of the individual algorithms (which are primarily estimates of the random uncertainty). This would in particular be important to get a handle on the systematic error component of the uncertainty, which is very difficult (if not impossible) to reliably quantify for each algorithm individually. For an ensemble, this would strictly speaking require that the median is bias free which is unlikely to be the case. Nevertheless, the spatio-temporal intervals where the various data products disagree are very likely intervals where the data products need to be used with care. In any case, reliable XCO₂ error estimates of the satellite retrievals are of critical importance for the user of the GHG-CCI atmospheric data products.

Figures such as Figure 6 also permits the determination of which of the data sets agree and which disagree. For example, the EMMA product, but also most of the individual TANSO products and SCIAMACHY/BESD, agree well or at least reasonably with each other as well as with TCCON and CarbonTracker (see green and yellow smileys), whereas this is not always true for the two very fast algorithms WFMD and PPDF (see red smileys). Figure 7 shows pie charts indicating the overall agreement and disagreement of each of the individual algorithms with the median. The results are consistent with the already reported findings, e.g., better performance of BESD compared to WFMD and similar performance of the TANSO XCO₂ algorithms.

A large number of other comparisons of the individual data products and the EMMA product with TCCON but also with CarbonTracker have been carried out. Figure 8 shows, as an example, a comparison of the amplitude of the XCO₂ seasonal cycle. As can be seen, all satellite data shown suggest that the seasonal cycle is underestimated by CarbonTracker by ~1.5 +/- 0.5 ppm peak-to-peak. Using only a single data product it would be difficult to “prove” that such a relatively small difference

(~0.3% of the total column) is significant and not caused by or at least significantly influenced by retrieval issues (see, e.g., the discussion given in Schneising et al., 2011, on this topic). Using an ensemble of data products based on more than one satellite and using several essentially independent algorithms allows one to draw more confident conclusions with respect to the interpretation of satellite – model XCO₂ differences than would be possible using a single data product only. Within GHG-CCI it is therefore planned to continue the efforts on EMMA in addition to further developing the individual algorithms.

5.4 Inter-comparison of SCIAMACHY XCH₄ data products

The multi-year global retrievals obtained from the two SCIAMACHY XCH₄ algorithms, WFMD and IMAP, have been compared with one another. Figure 9 shows, as a typical example, a comparison of one month (August 2005) of the global WFMD and IMAP data products (Figure 10 shows the corresponding results for July 2009; results for other months are shown in Buchwitz et al., 2012a). As can be seen, the monthly XCH₄ maps generated with the two algorithms show – depending on region – similar but also significantly different patterns. Both maps show higher methane concentrations over the Northern Hemisphere (NH), where most of the methane sources are located, compared to the Southern Hemisphere (SH). Both data sets agree reasonably well (within typically +/- 10 ppb) over most parts of the SH land areas but over some areas WFMD XCH₄ can be up to approximately 20 ppb higher. Over the NH the situation appears to be more complex. Both data sets show elevated methane over large parts of China, south-east Asia and India, but the patterns are not identical, with WFMD being higher over south-east Asia and lower over parts of India compared to IMAP. WFMD and IMAP not only use differently calibrated input data (standard versus non-standard calibration) and different retrieval methods (least squares versus OE), but also different post-processing quality filtering schemes. The latter is reflected by differences in spatial coverage (e.g., WFMD methane is not restricted to land observations only) and number of retrievals over a given region (see right hand side panels of Figure 9). The data density differs significantly depending on region. Typically WFMD has many more data points over the Sahara and other areas in the ~10°-40°N latitude range but also over mid/northern Australia and the mid/western part of the US, whereas IMAP has higher data

density over South America and mid/high northern latitudes. Large differences between the two data sets are also visible over large parts of northern Africa, where IMAP methane is higher (by approx. 40 ppb) and Greenland, where WFMD methane is higher (by approx. 40 ppb). The reasons for the differences have not yet been identified. It has also not yet been assessed to what extent inferred regional methane fluxes would differ depending on which data set is used as input data for inverse modeling of regional methane fluxes. Significant differences can be expected as the regional differences exceed the bias threshold requirement of less than 10 ppb. The discussion also shows that depending on region the differences can be significantly larger than the estimated biases listed in Table 5, which are based on the analysis of the satellite data at TCCON sites only. Clearly, more research is needed to understand the differences between the two SCIAMACHY methane data sets discussed in this section.

5.5 Inter-comparison of TANSO XCH₄ data products

Within GHG-CCI, four TANSO XCH₄ retrieval algorithms have been further developed and used to generate global data sets which have been inter-compared and compared with TCCON retrievals and global model data (Buchwitz et al., 2012a). The four retrieval algorithms are the FP and PR algorithms developed by SRON (SRFP, SRPR) and Univ. Leicester (UoL; OCFP and OCPR algorithms).

For the PR algorithms, which are based on the retrieval of ratios of the CH₄ to CO₂ columns, followed by a model-based CO₂ correction to compute XCH₄, the column ratios have been compared as well as the final XCH₄ product. As expected, it has been found that the agreement between the ratios is typically somewhat better compared to the XCH₄ products due to differences between the model-based CO₂ correction as used by SRON and UoL (see Buchwitz et al., 2012a, for details). Overall and in line with the discussion presented in Section 5.2, it has been found that the two PR products agree nearly equally well with the TCCON ground-based observations. A direct comparison of the two data products at TCCON sites is also shown in Figure 11 indicating agreement within typically 10 ppb (1-sigma). Nevertheless, inspection of global maps also reveals significant differences, depending on region and time. Qualitatively, this is similar to the results found for the SCIAMACHY data sets discussed in the previous section, but the differences shown in Figure 11 for TANSO are significantly

smaller compared to the differences for SCIAMACHY shown in Figures 9 and 10. Figure 11 shows a global OCPR-SRPR methane difference map for July 2009. As can be seen, the differences may exceed 5 ppb (breakthrough requirement) or even 10 ppb (threshold requirement) over certain extended regions such as India. Comparisons between the two FP TANSO XCH₄ data products OCFP and SRFP have also been carried out. Using SRFP, two years of global TANSO data have been retrieved but the comparison had to be limited to TCCON sites only because of limitations of the OCFP data set which is not yet available globally. It has been found that the inter-station bias is smaller for SRFP (~4 ppb) compared to OCFP (~8 ppb) and that the scatter of the SRFP data is somewhat smaller compared to the OCFP (14 ppb versus 16 ppb). These findings are consistent with the results presented in Table 5 but have been derived independently (see Buchwitz et al., 2012a). It has also been found that the agreement between the two PR algorithms is significantly better than the agreement between the two FP algorithms. This may be due to the fact that PR algorithms are simpler but may also indicate that at the current stage of development the PR algorithms are more mature (note that they also deliver much more data points, see Section 5.2).

5.6 Algorithm selection results

The main goal of the RR exercise was to determine which satellite retrieval algorithms to use to generate the CRDP. Based on the results presented and discussed in the previous sections, algorithms have been selected. The selection results are presented in the following sub-sections.

5.6.1 Selection results: SCIAMACHY and GOSAT XCO₂

Within GHG-CCI, two SCIAMACHY and two TANSO XCO₂ algorithms have been further developed and the corresponding data products have been inter-compared. They have also been compared with three other TANSO XCO₂ data products generated outside of this project: with the two TANSO XCO₂ products generated at NIES, Japan, (i.e., the operational TANSO product (Yoshida et al., 2011) and the scientific PPDF product (Oshchepkov et al., 2011)) and with the NASA ACOS team product (O'Dell et al., 2012, Crisp et al., 2012). Analysis of all seven products indicates that the precision requirement has been met, but not the very demanding bias requirement of less than 0.5 ppm

(approximately 1 ppm has been achieved at TCCON sites). Clearly, more work on the individual retrieval algorithms is required to achieve this goal and it has been decided to continue with all algorithms. A possible exception is the fast SCIAMACHY XCO₂ WFMD algorithm, which shows a reduced data quality in terms of precision and biases compared to the computationally much more demanding BESD algorithm. On the other hand the WFMD product has significantly (3-4 times) more data points compared to BESD and therefore much better coverage compared to any of the other data products including BESD. GHG-CCI aims at taking advantage of the fact that an ensemble of state-of-the-art data products exists which can be exploited. To this end, the EnSeMble Median Algorithm (EMMA) has been developed (Reuter et al., 2013). EMMA generates a Level 2 XCO₂ product using the median of the individual data products thereby largely eliminating outliers of the data products generated with the individual algorithms. EMMA may also improve the error characterization using the ensemble scatter. Preliminary analysis indicates that EMMA outperforms each of the individual algorithms. EMMA also permits the identification of potential weaknesses of the individual algorithms, which can be used to improve the individual algorithms. Taking this into account, it has been decided to proceed with all satellite XCO₂ algorithms and to add the EMMA data product to the GHG-CCI product portfolio.

5.6.2 Selection results: SCIAMACHY XCH₄

Data products generated with two algorithms have been assessed: WFMD (Schneising et al., 2011, 2012) and IMAP (Frankenberg et al., 2011). Comparison with ground-based TCCON observations revealed that both data products are very similar with respect to biases. This is also true for the estimated single measurement precisions for the time period 2003-2005, when the SCIAMACHY detector did not yet suffer from major degradation in the spectral region needed for methane retrieval. After 2005, the WFMD methane shows a larger scatter (~80 ppb) compared to IMAP (~50 ppb). Both data products have to be used with care for the time after 2005 due to potential bias issues related to detector degradation as indicated by the TCCON comparison at southern hemisphere TCCON sites, where both data products show a low bias of 20-30 ppb depending on FTS site. Considering only this

analysis, one would conclude that both data products are essentially equivalent and one may therefore select one of them. Analysis of spatially resolved global methane distributions as generated by the two algorithms however shows significant differences, depending on region and time, which are larger than the required maximum bias of 10 ppb, i.e., are significant for regional-scale methane surface flux inversions. Due to the lack of appropriate reference data such as TCCON, it was not yet possible to determine which of the two data products is the most accurate. Therefore, it has been decided to proceed with both algorithms and to contribute with both alternative data products to the CRDP pointing out the strength and weaknesses of the two approaches. Users will be encouraged to use both data sets, to determine to what extent their findings depend on the data product used, and to report these findings to the GHG-CCI retrieval experts.

5.6.3 Selection results: TANSO XCH₄

Four algorithms and their corresponding data products have been evaluated: OCFP and OCPR (Parker et al., 2011) and SRFP and SRPR (Butz et al., 2011). All data products show very similar biases and scatter when compared with ground-based TCCON observations. The number of data points is however significantly higher for the “Proxy” (PR) algorithms compared to the “Full Physics” (FP) algorithms and the agreement between the two PR data products is better than for the FP products, indicating a higher level of maturity of the (simpler) PR algorithms. Note that the SCIAMACHY XCH₄ algorithms, WFMD and IMAP, are also PR algorithms and that the FP algorithms are relatively new and currently in their early stages of development. Overall, the OCPR algorithm shows a slightly better performance compared to SRPR (primarily in terms of number of data points at TCCON sites). It has therefore been decided to continue with OCPR within GHG-CCI. The PR XCH₄ algorithms depend on a CO₂ correction using model data. The long-term goal of GHG-CCI is to use a FP algorithm that is independent of a CO₂ model. Because the SRFP algorithm shows a somewhat better performance compared to the OCFP algorithm (e.g., lower station-to-station biases at TCCON sites), it has been decided to continue with the SRFP algorithm, despite the lower number of data points compared to OCFP. In summary, four TANSO XCH₄ algorithms have been evaluated as part of

the GHG-CCI RR and two of these algorithms have been selected for further use within GHG-CCI:
OCPR and SRFP.

6. Additional Constraints Algorithms (ACAs)

The Additional Constraints Algorithms (ACAs) are algorithms to retrieve CO₂ and/or CH₄ information for layers above the planetary boundary layer. ACAs are applied to several satellite instruments. An overview of the ACAs used within GHG-CCI is given in Table 3. As the ACAs are not the focus of this manuscript the reader is referred to the references listed in Table 3 (including caption) for details on each of these algorithms and corresponding data products.

For ACAs only one algorithm per data product has been considered within GHG-CCI, i.e., ACAs are also being further developed but not in competition and not by covering all aspects (e.g., no dedicated validation). For ACAs a number of criteria have been defined which need to be fulfilled to contribute to the CRDP but detailed user requirements have not been formulated.

Only a limited assessment of the data products generated with ACAs has been conducted during the initial phase of GHG-CCI described in this manuscript because the focus was on ECAs. However, for each of the ACAs listed in Table 3 it has been determined if the selection criteria specified in the Round Robin Evaluation Procedure (RREP, Buchwitz et al., 2011b) have been met. The RREP defines 11 criteria for ACAs which need to be fulfilled for a given ACA to contribute to the CRDP. The criteria are mostly qualitative and refer to a required minimum level of documentation, error analysis and related auxiliary information. All ACA products are potentially useful for GHG-CCI climate applications as they deliver additional information on CO₂ and/or CH₄ thereby providing potentially important constraints when used, for example, within an appropriate inverse modeling framework to derive regional surface fluxes from the satellite observations. However, no detailed user requirements are currently available, no dedicated validation has been performed within GHG-CCI and it has also not been assessed to what extent the existing products are useful or not useful for GHG surface flux inverse modeling. More research is needed to assess the usefulness of these data products for climate

relevant applications. It has been identified that all ACAs fulfill the requirements listed in the RREP and that all ACA products can therefore be included in the CRDP.

7. Climate Research Data Package (CRDP)

The goal of the GHG-CCI RR was to decide which algorithms to use to generate the CRDP. It is planned to generate the CRDP during September 2012 to March 2013. Table 6 presents an overview of the planned content of the CRDP in terms of data products and their spatio-temporal coverage. The CRDP will contain all relevant information needed for inverse modeling such as single observation uncertainties, *a priori* profiles and averaging kernels. The CRDP will be validated during March-May 2013 and subsequently evaluated by the GHG-CCI users (June-August 2013). By the end of August, the CRDP along with the corresponding documentation will be made publicly available via the GHG-CCI website.

8. Summary and conclusions

An overview of the main activities and results achieved during the first two years of the GHG-CCI project of ESA's Climate Change Initiative (CCI) has been presented, focusing on the CCI "Round Robin" (RR) exercise. The goal of CCI is to generate a number of Essential Climate Variables (ECVs) in-line with GCOS (Global Climate Observing System) requirements and guidelines using European Earth observation data and data from ESA Third Party Missions (TPM) such as GOSAT. To achieve this, several existing state-of-the-art retrieval algorithms for retrieving XCO₂ and XCH₄ from SCIAMACHY/ENVISAT and TANSO/GOSAT nadir radiance spectra have been further improved in order to meet challenging requirements for the targeted regional CO₂ and CH₄ surface flux (source/sink) application as defined by the GHG-CCI Climate Research Group (CRG). The ultimate goal of the RR was to identify and select the best algorithms to be used for generating the Climate Research Data Package (CRDP), which will essentially be the first version of the CCI ECV GHG data base. In addition, retrieval algorithms for a number of other satellite instruments such as IASI and MIPAS have also been further developed, but not in competition.

Substantial progress has been made during the first two years (September 2010 – August 2012) of the GHG-CCI project. For example, longer XCO₂ and XCH₄ time series have been generated from SCIAMACHY with improved data quality and better error characterization (Reuter et al., 2011, Frankenberg et al., 2011, Schneising et al., 2011, 2012, Heymann et al., 2012a, 2012b). The same is true for TANSO (Butz et al., 2011, Parker et al., 2011, Schepers et al., 2012, Cogan et al., 2012).

Several retrieval algorithms have been further developed in competition during the GHG-CCI RR and used to generate global multi-year data sets of XCO₂ and XCH₄ from SCIAMACHY and TANSO. The data products have been evaluated by comparison with ground-based TCCON observations, by inter-comparisons of the data products generated with the different candidate algorithms, and by comparisons with other data sets including global models. Due to the sparseness of the TCCON network it was not planned to base the algorithm selection decision only on satellite – TCCON comparisons. It has been found that nearly all candidate algorithms produce data with very similar quality at TCCON sites, i.e., show similar satellite – TCCON differences. Significant differences have however been found remote from TCCON when comparing the global data sets, e.g., when comparing global maps. Depending on region and time, it has been found that the differences may exceed the systematic error requirements of less than 0.5 ppm for XCO₂ and 10 ppb for XCH₄. It has been identified that more research is needed in order to understand the differences between the various data sets. It was therefore not possible for all products to clearly identify which of the candidate algorithms performs best. The goal of the RR was to identify which of the competing algorithms to use for the CRDP. The selected algorithms are listed in Table 6. A summary of the RR algorithm selection decision and justification is given in Section 5.6 for the GHG-CCI ECV core data products and in Section 6 for additional products generated with algorithms not in competition during the RR phase.

The climate and inverse modeling community requires long-term datasets of near-surface-sensitive CO₂ and CH₄ observations that are as accurate and precise as possible. The goal of GHG-CCI is to build up such a time series starting with SCIAMACHY/ENVISAT (March 2002 – April 2012) and being continued with GOSAT (launch 2009) and future GHG satellite missions such as OCO-2 (Boesch et al., 2011), Sentinel-5-Precursor (Butz et al., 2012) and potentially CarbonSat

(Bovensmann et al., 2010). As shown in this manuscript, significant progress has been made to achieve this goal, but more work is needed in order to meet the demanding user requirements for as many conditions as possible.

9. Acknowledgements

This work was primarily funded by ESA/ESRIN (GHG-CCI) but also received funding from EU FP7 (grant agreement No. 283576, MACC-II), DLR (SADOS), and the State and the University of Bremen. We thank the members of the GOSAT Project (JAXA, NIES, and Ministry of the Environment (MoE), Japan) for providing GOSAT Level 1B and Level 2 data products (GOSAT RA1 PI project CONSCIGO). The ACOS v2.9 data were produced by the ACOS/OCO-2 project at the Jet Propulsion Laboratory, California Institute of Technology, and obtained from the ACOS/OCO-2 data archive maintained at the NASA Goddard Earth Science Data and Information Services Center. We thank NOAA for making available the CarbonTracker CO₂ fields. We also thank TCCON and related funding organizations (NASA grants NNX11AG01G, NAG5-12247, NNG05-GD07G, NASA Orbiting Carbon Observatory Program, DOE ARM program, the Australian Research Council, DP0879468 and LP0562346, the EU projects IMECC and GEOmon, the Senate of Bremen). Last but not least we would like to thank the two referees for helpful comments.

841

842 **10. References**

843 Bergamaschi, P., Frankenberg, C., Meirink, J.F., Krol, M., Dentener, F., Wagner, T., Platt, U., Kaplan,
844 J.O., Körner, S., Heimann, M., Dlugokencky, E.J., Goede, A. (2007), Satellite cartography of
845 atmospheric methane from SCIAMACHY onboard ENVISAT: 2. Evaluation based on inverse
846 model simulations, *J. Geophys. Res.*, 112, D02304, doi:10.1029/2006JD007268.

847 Bergamaschi, P., Frankenberg, C., Meirink, J. F., Krol, M., Villani, M. G., Houweling, S., Dentener,
848 F., Dlugokencky, E. J., Miller, J. B., Gatti, L. V., Engel, A., Levin, I. (2009), Inverse modeling
849 of global and regional CH₄ emissions using SCIAMACHY satellite retrievals, *J. Geophys.*
850 *Res.*, 114, D22301, doi:10.1029/2009JD01228.

851 Bloom, A. A., Palmer, P. I., Fraser, A., Reay, D. S., Frankenberg, C. (2010), Large-scale controls of
852 methanogenesis inferred from methane and gravity spaceborne data, *Science*, 327, 322–325,
853 doi:10.1126/science.1175176.

854 Boesch, H., Baker, D., Connor, B., Crisp, D., Miller, C. (2011): Global Characterization of CO₂
855 Column Retrievals from Shortwave-Infrared Satellite Observations of the Orbiting Carbon
856 Observatory-2 Mission, *Remote Sens.*, 3, 270–304, doi:10.3390/rs3020270,
857 <http://www.mdpi.com/2072-4292/3/2/270/> .

858 Bovensmann, H., Burrows, J. P., Buchwitz, M., Frerick, J., Noël, S., Rozanov, V. V., Chance, K. V.,
859 Goede, A. H. P. (1999), SCIAMACHY - Mission objectives and measurement modes, *J.*
860 *Atmos. Sci.*, 56 (2), 127-150.

861 Bovensmann, H., Buchwitz, M., Burrows, J. P., Reuter, M., Krings, T., Gerilowski, K., Schneising, O.,
862 Heymann, J., Tretner, A., Erzinger, J. (2010), A remote sensing technique for global
863 monitoring of power plant CO₂ emissions from space and related applications, *Atmos. Meas.*
864 *Tech.*, 3, 781-811.

865 Bril, A., Oshchepkov, S., Yokota, T., Inoue, G. (2007): Parameterization of aerosol and cirrus cloud
 866 effects on reflected sunlight spectra measured from space: application of the equivalence
 867 theorem, *Appl. Opt.*, Vol.46(13), 2460-2470.

868 Buchwitz, M., Rozanov, V. V., Burrows, J. P. (2000), A near-infrared optimized DOAS method for
 869 the fast global retrieval of atmospheric CH₄, CO, CO₂, H₂O, and N₂O total column amounts
 870 from SCIAMACHY Envisat-1 nadir radiances, *J. Geophys. Res.*, 105, 15,231-15,245.

871 Buchwitz, M., de Beek, R., Burrows, J. P., Bovensmann, H., Warneke, T., Notholt, J., Meirink, J. F.,
 872 Goede, A. P. H., Bergamaschi, P., Körner, S., Heimann, M., Schulz, A. (2005), Atmospheric
 873 methane and carbon dioxide from SCIAMACHY satellite data: Initial comparison with
 874 chemistry and transport models, *Atmos. Chem. Phys.*, 5, 941-962.

875 Buchwitz, M., Schneising, O., Burrows, J. P., Bovensmann, H., Reuter, M., Notholt, J. (2007), First
 876 direct observation of the atmospheric CO₂ year-to-year increase from space, *Atmos. Chem.*
 877 *Phys.*, 7, 4249-4256.

878 Buchwitz, M., Chevallier, F., Bergamaschi, P. (2011a), User Requirements Document (URD) for the
 879 GHG-CCI project of ESA's Climate Change Initiative, Technical Report, pp. 45, version 1
 880 (URDv1), 3. February 2011, available from <http://www.esa-ghg-cci.org>.

881 Buchwitz, M., Reuter, M., Chevallier, F., Bergamaschi, P. (2011b), Round Robin Evaluation Protocol
 882 (RREP) for the GHG-CCI project of ESA's Climate Change Initiative, Technical Report, pp.
 883 15, version 2 (RREPV2), 17. August 2011, available from <http://www.esa-ghg-cci.org>.

884 Buchwitz, M., Reuter, M., Schneising, O., Parker, R., Guerlet, Noël, S., S. Crevoisier, C., Laeng, A.
 885 (2011c), Algorithm Inter-comparison and Error Characterization & Analysis Report
 886 (AIECAR) of the GHG-CCI project of ESA's Climate Change Initiative, Technical Report,
 887 pp. 192, version 0 (AIECARv0), 22. August 2011, available from <http://www.esa-ghg-cci.org>.

888 Buchwitz, M., Reuter, M., Schneising, O., Parker, R., Guerlet, Noël, S., S. Crevoisier, C., Laeng, A.
 889 (2012a), Algorithm Inter-comparison and Error Characterization & Analysis Report

890 (AIECAR) of the GHG-CCI project of ESA's Climate Change Initiative, Technical Report,
891 version 1 (AIECARv1), 28. August 2012, available from <http://www.esa-ghg-cci.org>.

892 Buchwitz, M., Chevallier, F., Bergamaschi, P., Kaminski, T. (2012b), Algorithm Selection Report
893 (ASR) of the GHG-CCI project of ESA's Climate Change Initiative, Technical Report, 29.
894 August 2012, available from <http://www.esa-ghg-cci.org>.

895 Butz, A., Guerlet, S., Hasekamp, O., Schepers, D., Galli, A., Aben, I., Frankenberg, C., Hartmann, J.-
896 M., Tran, H., Kuze, A., Keppel-Aleks, G., Toon, G., Wunch, D., Wennberg, P., Deutscher,
897 N., Griffith, D., Macatangay, R., Messerschmidt, J., Notholt, J., Warneke, T. (2011),
898 Towards accurate CO₂ and CH₄ observations from GOSAT, *Geophys. Res. Lett.*,
899 doi:10.1029/2011GL047888.

900 Butz, A., Galli, A., Hasekamp, O., Landgraf, J., Tol, J. P., Aben, I. (2012), TROPOMI aboard
901 Sentinel-5 Precursor: Prospective performance of CH₄ retrievals for aerosol and cirrus loaded
902 atmospheres, *Remote Sensing of Environment*, 120, 267 – 276.

903 Canadell, J. G., Ciais, P., Dhakal, S., Dolman, H., Friedlingstein, P., Gurney, K. R., Held, A., Jackson,
904 R. B., Le Quéré, C., Malone, E. L., Ojima, D. S., Patwardhan, A., Peters, G. P., Raupach, M.
905 R. (2010), Interactions of the carbon cycle, human activity, and the climate system: a research
906 portfolio, *Current Opinion in Environmental Sustainability*, 2, 301–311, available online at
907 www.sciencedirect.com.

908 Chevallier, F., Engelen, R. J., Peylin, P. (2005), The contribution of AIRS data to the estimation of
909 CO₂ sources and sinks. *Geophys. Res. Lett.*, 32, L23801, doi:10.1029/2005GL024229.

910 Chevallier, F., Bréon, F.-M., and Rayner, P. J. (2007), Contribution of the Orbiting Carbon
911 Observatory to the estimation of CO₂ sources and sinks: Theoretical study in a variational data
912 assimilation framework, *J. Geophys. Res.*, 112, D09307, doi:10.1029/2006JD007375.

913 Cogan, A., Boesch, H., Parker, R., Feng, L., Palmer, P., Blavier, J.-F., Deutscher, N., Macatangay, R.,
914 Notholt, J., Roehl, C. M., Warneke, T., Wunch, D. (2012), Atmospheric carbon dioxide
915 retrieved from the Greenhouse gases Observing SATellite: Comparison with ground-based

916 TCCON observations and GEOS-Chem model calculations, *J. Geophys. Res.*, 117, D21,
 917 doi:10.1029/2012JD018087.

918 Crevoisier, C., Heilliette, S., Chédin, A., Serrar, S., Armante, R., Scott, N.A. (2004), Midtropospheric
 919 CO₂ concentration retrieval from AIRS observations in the tropics, *Geophys. Res. Lett.*, 31,
 920 L17106, doi:10.1029/2004GL020141.

921 Crevoisier, C., Chédin, A., Matsueda, H., Machida, T., Armante, R., Scott, N. A. (2009a), First year of
 922 upper tropospheric integrated content of CO₂ from IASI hyperspectral infrared observations,
 923 *Atmos. Chem. Phys.*, 9, 4797–4810.

924 Crevoisier, C., Nobileau, D., Fiore, A., Armante, R., Chédin, A., Scott, N. A. (2009b), Tropospheric
 925 methane in the tropics – first year from IASI hyperspectral infrared observations, *Atmos.*
 926 *Chem. Phys.*, 9, 6337–6350.

927 Crisp, D., Atlas, R. M., Bréon, F.-M., Brown, L. R., Burrows, J. P., Ciais, P., Connor, B. J., Doney, S.
 928 C., Fung, I. Y., Jacob, D. J., Miller, C. E., O'Brien, D., Pawson, S., Randerson, J. T., Rayner,
 929 P., Salawitch, R. S., Sander, S. P., Sen, B., Stephens, G. L., Tans, P. P., Toon, G. C.,
 930 Wennberg, P. O., Wofsy, S. C., Yung, Y. L., Kuang, Z., Chudasama, B., Sprague, G., Weiss,
 931 P., Pollock, R., Kenyon, D., Schroll, S. (2004), The Orbiting Carbon Observatory (OCO)
 932 mission, *Adv. Space Res.*, 34, 700-709.

933 Crisp, D., Fisher, B. M., O'Dell, C., Frankenberg, C., Basilio, R., Boesch, H. L. R. Brown, R.
 934 Castano, B. Connor, N. M. Deutscher, A. Eldering, D. Griffith, M. Gunson, A. Kuze, L.
 935 Mandrake, J. McDuffie, J. Messerschmidt, C. E. Miller, I. Morino, V. Natraj, J. Notholt, D. M.
 936 O'Brien, F. Oyafuso, I. Polonsky, J. Robinson, R. Salawitch, V. Sherlock, M. Smyth, H. Suto,
 937 T. E. Taylor, D. R. Thompson, P. O. Wennberg, D. Wunch, Y. L. Yung (2012), The ACOS CO₂
 938 retrieval algorithm – Part II: Global XCO₂ data characterization, *Atmos. Meas. Tech.*, 5, 687–
 939 707.

940 Deutscher, N. M., Griffith, D. W. T., Bryant, G. W., Wennberg, P. O., Toon, G. C., Washenfelder, R.
 941 A., Keppel-Aleks, G., Wunch, D., Yavin, Y. G., Allen, N. T., Blavier, J.-F. L., Jiménez, R.,

942 Daube, B. C., Bright, A. V, Matross, D. M., Wofsy, S. C., Park, S. (2010), Total column CO₂
 943 measurements at Darwin, Australia – site description and calibration against in situ aircraft
 944 profiles, *Atmos. Meas. Tech.*, 3(4), 947–958, doi:10.5194/amt-3-947-2010.

945 Dlugokencky, E. J., Bruhwiler, L., White, J. W. C., Emmons, L. K., Novelli, P. C., Montzka, S. A.,
 946 Masarie, K. A., Lang, P. M., Crotwell, A. M., Miller, J. B., Gatti, L. V. (2009), Observational
 947 constraints on recent increases in the atmospheric CH₄ burden, *Geophys. Res. Lett.*, 36,
 948 L18803, doi:10.1029/2009GL039780.

949 Sussmann, R., Ostler, A., Forster, F., Rettinger, M., Deutscher, N. M., Griffith, D. W. T., Hannigan, J.
 950 W., Jones, N., Patra, P. K. (2013), First intercalibration of column-averaged methane from the
 951 Total Carbon Column Observing Network and the Network for the Detection of Atmospheric
 952 Composition Change, *Atmos. Meas. Tech.*, 6, 397–418.

953 Foucher, P. Y., Chédin, A., Dufour, G., Capelle, V., Boone, C. D., Bernath, P. (2009), Technical Note:
 954 Feasibility of CO₂ profile retrieval from limb viewing solar occultation made by the ACE-FTS
 955 instrument, *Atmos. Chem. Phys.*, 9, 2873–2890.

956 Frankenberg, C., Meirink, J. F., van Weele, M., Platt, U., Wagner, T. (2005), Assessing methane
 957 emissions from global spaceborne observations, *Science*, 308, 1010–1014.

958 Frankenberg, C., Aben, I., Bergamaschi, P., Dlugokencky, E. J., van Hees, R., Houweling, S., van der
 959 Meer, P., Snel, R., Tol, P. (2011), Global column-averaged methane mixing ratios from 2003
 960 to 2009 as derived from SCIAMACHY: Trends and variability, *J. Geophys. Res.*,
 961 doi:10.1029/2010JD014849.

962 GCOS (Global Climate Observing System) (2006), Systematic Observation Requirements for
 963 Satellite-based products for Climate – Supplemental Details to the GCOS Implementation
 964 Plan, GCOS 107, September 2006.

965 Geibel, M. C., Messerschmidt, J., Gerbig, C., Blumenstock, T., Chen, H., Hase, F., Kolle, O., Lavric,
 966 J. V., Notholt, J., Palm, M., Rettinger, M., Schmidt, M., Sussmann, R., Warneke, T., Feist, D.
 967 G. (2012), Calibration of column-averaged CH₄ over European TCCON FTS sites with

968 airborne in-situ measurements, *Atmos. Chem. Phys.*, 12, 8763–8775, doi:10.5194/acp-12-
 969 8763-2012.

970 Heymann, J., Schneising, O., Reuter, M., Buchwitz, M., Rozanov, V. V., Velazco, V. A.,
 971 Bovensmann, H., Burrows, J. P. (2012a), SCIAMACHY WFM-DOAS XCO₂: comparison
 972 with CarbonTracker XCO₂ focusing on aerosols and thin clouds, *Atmos. Meas. Tech.*, 5, 1935-
 973 1952, 2012.

974 Heymann, J., Bovensmann, H., Buchwitz, M., Burrows, J. P., Deutscher, N. M., Notholt, J., Rettinger,
 975 M., Reuter, M., Schneising, O., Sussmann, R., Warneke, T. (2012b), SCIAMACHY WFM-
 976 DOAS XCO₂: reduction of scattering related errors, *Atmos. Meas. Tech.*, 5, 2375-2390, 2012.

977 Kaminski, T., Scholze, M., Houweling, S. (2010), Quantifying the Benefit of A-SCOPE
 978 Data for Reducing Uncertainties in Terrestrial Carbon Fluxes in CCDAS. *Tellus B*,
 979 doi:10.1111/j.1600-0889.2010.00483.x

980 Kaminski, T., Knorr, W., Scholze, M., Gobron, N., Pinty, R., Giering, R., Mathieu, P.-P. (2012),
 981 Consistent Assimilation of MERIS FAPAR and atmospheric CO₂ into a Terrestrial Vegetation
 982 Model and Interactive Mission Benefit Analysis. *Biogeosciences*, 9(8):3173-3184.

983 Knutti, R., R. Furrer, C. Tebaldi, J. Cermak, G. A. Meehl (2010), Challenges in Combining
 984 Projections from Multiple Climate Models. *J. Climate*, 23, 2739–2758. doi:
 985 <http://dx.doi.org/10.1175/2009JCLI3361.1>

986 Kuze, A., Suto, H., Nakajima, M., and Hamazaki, T. (2009), Thermal and near infrared sensor for
 987 carbon observation Fourier-transform spectrometer on the Greenhouse Gases Observing
 988 Satellite for greenhouse gases monitoring, *Appl. Opt.*, 48, 6716–6733.

989 Meirink, J. F., Eskes, H. J., and Goede, A. P. H. (2006), Sensitivity analysis of methane emissions
 990 derived from SCIAMACHY observations through inverse modelling, *Atmos. Chem. Phys.*, 6,
 991 1275–1292.

992 Messerschmidt, J., Geibel, M. C., Blumenstock, T., Chen, H., Deutscher, N. M., Engel, A., Feist, D.
 993 G., Gerbig, C., Gisi, Hase, M. F., Katrynski, K., Kolle, O., Lavric, J. V., Notholt, J., Palm, M.,

994 Ramonet, M., Rettinger, M., Schmidt, M., Sussmann, R., Toon, G. C., F. Truong, F., Warneke,
 995 T., Wennberg, P. O., Wunch, D., Xueref-Remy, I. (2012), Calibration of TCCON column-
 996 averaged CO₂: the first aircraft campaign over European TCCON sites, *Atmos. Chem. Phys.*,
 997 11, 10765-10777.

998 Noël, S., Bramstedt, K., Rozanov, A., Bovensmann, H., Burrows, J. P. (2011), Stratospheric methane
 999 profiles from SCIAMACHY solar occultation measurements derived with onion peeling
 1000 DOAS, *Atmos. Meas. Tech.*, 4, 2567-2577.

1001 Notholt, J., Dils, B., Blumenstock, T., Brunner, D., Buchmann, B., De Mazière, M., Popp, C.,
 1002 Sussmann, R. (2012), Product Validation and Algorithm Selection Report (PVASR) of the
 1003 GHG-CCI project of ESA's Climate Change Initiative, Technical Report, 22. August 2012,
 1004 available from <http://www.esa-ghg-cci.org>.

1005 O'Dell, C. W., Connor, B., Boesch, H., O'Brien, D., Frankenberg, C., Castano, R., Christi, M.,
 1006 Eldering, D., Fisher, B., Gunson, M., McDuffie, J., Miller, C. E., Natraj, V., Oyafuso, F.,
 1007 Polonsky, I., Smyth, M., Taylor, T., Toon, G. C., Wennberg, P. O., Wunch, D., (2012), The
 1008 ACOS CO₂ retrieval algorithm – Part 1: Description and validation against synthetic
 1009 observations, *Atmos. Meas. Tech.*, 5, 99–121, 2012.

1010 Oshchepkov S., Bril, A., Yokota, T. (2008), PPDF-based method to account for atmospheric light
 1011 scattering in observations of carbon dioxide from space. *J. Geophys. Res.*, 113, D23210.

1012 Oshchepkov S., Bril, A., Yokota, T. (2009), An improved photon path length probability density
 1013 function-based radiative transfer model for space-based observation of greenhouse gases. *J.*
 1014 *Geophys. Res.*, 114, D19207.

1015 Oshchepkov, S., Bril, A., Maksyutov, S., Yokota, T. (2011), Detection of optical path in spectroscopic
 1016 space-based observations of greenhouse gases: Application to GOSAT data processing, *J.*
 1017 *Geophys. Res.*, 116, D14304, doi:10.1029/2010JD015352.

1018 Oshchepkov, S., Bril, A., Yokota, T., Morino, I., Yoshida, Y., Matsunaga, T., Belikov, D., Wunch, D.,
 1019 Wennberg, P., Toon, G., O'Dell, C., Butz, A., Guerlet, S., Cogan, A., Boesch, H., Eguchi, N.,
 1020 Deutscher, N., Griffith, G., Macatangay, R., Notholt, J., Sussmann, R., Rettinger, M.,

1021 Sherlock, V., Robinson, J., Kyrö, E., Heikkinen, P., Feist, D. G., Nagahama, T., Kadygrov, N.,
 1022 Maksyutov, S., Uchino, O., Watanabe, H. (2012), Effects of atmospheric light scattering on
 1023 spectroscopic observations of greenhouse gases from space: Validation of PPDF-based CO₂
 1024 retrievals from GOSAT, *J. Geophys. Res.*, 117, D12305, doi:10.1029/2012JD017505.

1025 Parker, R., Boesch, H., Cogan, A., Fraser, A., Feng, L., Palmer, P., Messerschmidt, J., Deutscher, N.,
 1026 Griffith, D., Notholt, J., Wennberg, P. Wunch, D. (2011), Methane Observations from the
 1027 Greenhouse gases Observing SATellite: Comparison to ground-based TCCON data and Model
 1028 Calculations, *Geophys. Res. Lett.*, doi:10.1029/2011GL047871.

1029 Peters, W., Jacobson, A. R., Sweeney, C., Andrews, A. E., Conway, T. J., Masarie, K., Miller, J. B.,
 1030 Bruhwiler, L. M. P., Petron, G., Hirsch, A. I., Worthy, D. E. J., van der Werf, G. R.,
 1031 Randerson, J. T., Wennberg, P. O., Krol, M. C., Tans, P. P. (2007): An atmospheric
 1032 perspective on North American carbon dioxide exchange: CarbonTracker, Proceedings of the
 1033 National Academy of Sciences (PNAS) of the United States of America, 27 Nov. 2007,
 1034 104(48), 18925-18930.

1035 Reuter, M., Buchwitz, M., Schneising, O., Heymann, J., Bovensmann, H., Burrows, J. P. (2010), A
 1036 method for improved SCIAMACHY CO₂ retrieval in the presence of optically thin clouds,
 1037 *Atmos. Meas. Tech.*, 3, 209-232.

1038 Reuter, M., Bovensmann, H., Buchwitz, M., Burrows, J. P., Connor, B. J., Deutscher, N. M., Griffith,
 1039 D. W. T., Heymann, J., Keppel-Aleks, G., Messerschmidt, J., Notholt, J., Petri, C., Robinson,
 1040 J., Schneising, O., Sherlock, V., Velasco, V., Warneke, T., Wennberg, P. O., Wunch, D.
 1041 (2011), Retrieval of atmospheric CO₂ with enhanced accuracy and precision from
 1042 SCIAMACHY: Validation with FTS measurements and comparison with model results, *J.*
 1043 *Geophys. Res.*, 116, D04301, doi:10.1029/2010JD015047.

1044 Reuter, M., Schneising, O., Parker, R., Guerlet, S., Noël, S., Crevoisier, C., Laeng, A. (2012a),
 1045 Algorithm Theoretical Basis Document (ATBD) of the GHG-CCI project of ESA's Climate
 1046 Change Initiative, Technical Report, pp. 486, version 1 (ATBDv1), 15. March 2012, available
 1047 from <http://www.esa-ghg-cci.org>.

1048 Reuter, M., Buchwitz, M., Schneising, O., Hase, F., Heymann, J., Guerlet, S., Cogan, A. J.,
 1049 Bovensmann, H., Burrows, J. P., (2012b), A simple empirical model estimating atmospheric
 1050 CO₂ background concentrations, *Atmos. Meas. Tech.*, 5, 1349-1357.

1051 Reuter, M., Boesch, H., Bovensmann, H., Bril, A., Buchwitz, M., Butz, A., Burrows, J. P., O'Dell, C.
 1052 W., Guerlet, S., Hasekamp, O., Heymann, J., Kikuchi, S. Oshchepkov, S., Parker, R., Pfeifer,
 1053 S., Schneising, O., Yokota, T., Yoshida, Y. (2013), A joint effort to deliver satellite retrieved
 1054 atmospheric CO₂ concentrations for surface flux inversions: The ensemble median algorithm
 1055 EMMA, *Atmos. Chem. Phys.*, 13, 1771-1780.

1056 Rigby, M., Prinn, R. G., Fraser, P. J., Simmonds, P. G., Langenfelds, R. L., Huang, J., Cunnold, D. M.,
 1057 Steele, L. P., Krummel, P. B., Weiss, R. F., O'Doherty, S., Salameh, P. K., Wang, H. J., Harth,
 1058 C. M., Mühle, J., Porter, L. W. (2008), Renewed growth of atmospheric methane, *Geophys.*
 1059 *Res. Lett.*, 35, L22805, doi:10.1029/2008GL036037.

1060 Rodgers, C. D. (2000), Inverse Methods for Atmospheric Sounding: Theory and Practice, *World*
 1061 *Scientific Publishing*.

1062 Schepers, D., Guerlet, S., Butz, A., Landgraf, J., Frankenberg, C., Hasekamp, O., Blavier, J.-F.,
 1063 Deutscher, N. M., Griffith, D. W. T., Hase, F., Kyro, E., Morino, I., Sherlock, V., Sussmann,
 1064 R., Aben, I. (2012), Methane retrievals from Greenhouse Gases Observing Satellite (GOSAT)
 1065 shortwave infrared measurements: Performance comparison of proxy and physics retrieval
 1066 algorithms, *J. Geophys. Res.*, 117, D10307, doi:10.1029/2012JD017549.

1067 Schneising, O., Buchwitz, M., Burrows, J. P., Bovensmann, H., Reuter, M., Notholt, J., Macatangay,
 1068 R., Warneke, T. (2008), Three years of greenhouse gas column-averaged dry air mole
 1069 fractions retrieved from satellite - Part 1: Carbon dioxide, *Atmos. Chem. Phys.*, 8, 3827-3853,
 1070 2008.

1071 Schneising, O., Buchwitz, M., Burrows, J. P., Bovensmann, H., Bergamaschi, P., Peters, W. (2009),
 1072 Three years of greenhouse gas column-averaged dry air mole fractions retrieved from satellite
 1073 - Part 2: Methane, *Atmos. Chem. Phys.*, 9, 443-465.

1074 Schneising, O., Buchwitz, M., Reuter, M., Heymann, J., Bovensmann, H., and Burrows, J. P. (2011),
 1075 Long-term analysis of carbon dioxide and methane column-averaged mole fractions retrieved
 1076 from SCIAMACHY, *Atmos. Chem. Phys.*, 11, 2881-2892.

1077 Schneising, O., Bergamaschi, P., Bovensmann, H., Buchwitz, M., Burrows, J. P., Deutscher, N. M.,
 1078 Griffith, D. W. T., Heymann, J., Macatangay, R., Messerschmidt, J., Notholt, J., Rettinger, M.,
 1079 Reuter, M., Sussmann, R., Velazco, V. A., Warneke, T., Wennberg, P. O., Wunch, D. (2012),
 1080 Atmospheric greenhouse gases retrieved from SCIAMACHY: comparison to ground-based
 1081 FTS measurements and model results, *Atmos. Chem. Phys.*, 12, 1527-1540.

1082 Simpson, I. J., Sulbaek Andersen, M. P., Meinardi, S., Bruhwiler, L., Blake, N. J., Helmig, D.,
 1083 Rowland, F. S., Blake, D. R. (2012), Long-term decline of global atmospheric ethane concentrations
 1084 and implications for methane, *Nature*, www.nature.com/doi/10.1038/nature11342

1085 Solomon, S., Qin, D., Manning, M., Chen, Z., Marquis, M., Averyt, K. B., Tignor, M., and Miller, H.
 1086 L. (Eds.): Climate Change 2007: The Physical Science Basis, Contribution of Working Group
 1087 I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC),
 1088 Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, 2007.

1089 Stephens, B. B., Gurney, K. R., Tans, P. P., Sweeney, C., Peters, W., Bruhwiler, L., Ciais, P.,
 1090 Ramonet, M., Bousquet, P., Nakazawa, T., Aoki, S., Machida, T., Inoue, G., Vinnichenko, N.,
 1091 Lloyd, J., Jordan, A., Heimann, M., Shibistova, O., Langenfelds, R. L., Steele, L. P., Francey,
 1092 R. J., and Denning, A. S. (2007), Weak northern and strong tropical land carbon uptake from
 1093 vertical profiles of atmospheric CO₂, *Science*, 316, 1732–1735.

1094 Toon, G. (1991), The JPL MkIV interferometer, *Optics Photonics News*, 2, 19–21.

1095 von Clarmann, T., Höpfner, M., Kellmann, S., Linden, A., Chauhan, S., Funke, B., Grabowski, U.,
 1096 Glatthor, N., Kiefer, M., Schieferdecker, T., Stiller, G., Versick, S. (2009), Retrieval of
 1097 temperature, H₂O, O₃, HNO₃, CH₄, N₂O, ClONO₂ and ClO from MIPAS reduced resolution
 1098 nominal mode limb emission measurements, *Atmos. Meas. Tech.*, 2, 159-175.

1099 Wecht, K. J., Jacob, D. J., Wofsy, S. C., Kort, E. A., Worden, J. R., Kulawik, S. S., Henze, D. K., M.
 1100 Kopacz, M., H. Payne, V. H. (2012), Validation of TES methane with HIPPO aircraft

1101 observations: implications for inverse modeling of methane sources, *Atmos. Chem. Phys.*, 12,
 1102 1823–1832.

1103 Wofsy, S. C., Daube, B. C., Jimenez, R., Kort, E., Pittman, J. V., Park, S., Commane, R., Xiang, B.,
 1104 Santoni, G., Jacob, D., Fisher, J., Pickett-Heaps, C., Wang, H., Wecht, K., Wang, Q.-Q.,
 1105 Stephens, B. B., Schertz, S., Romashkin, P., Campos, T., Haggerty, J., Cooper, W. A., Rogers,
 1106 D., Beaton, S., Elkins, J. W., Fahey, D., Gao, R., Moore, F., Montzka, S. A., Schwartz, J. P.,
 1107 Hurst, D., Miller, B., Sweeney, C., Oltmans, S., Nance, D., Hints, E., Dutton, G., Watts, L.
 1108 A., Spackman, R., Rosenlof, K., Ray, E., Zondlo, M., Diao, M., Mahoney, M. J., Chahine, M.,
 1109 Olsen, E., Keeling, R., Bent, J., Atlas, E. A., Lueb, R., Patra, P., Ishijima, K., Engelen, R.,
 1110 Nassar, R., Jones, D. B., Mikaloff-Fletcher, S. (2011), HIAPER Pole-to-Pole Observations
 1111 (HIPPO): Fine grained, global scale measurements for determining rates for transport, surface
 1112 emissions, and removal of climatically important atmospheric gases and aerosols, *Philos. T.*
 1113 *Roy. Soc. A*, 369, 2073–2086, doi:10.1098/rsta.2010.0313, 2011.

1114 Wunch, D., Toon, G. C., Wennberg, P. O., Wofsy, S. C., Stephens, B. B., Fischer, M. L., Uchino, O.,
 1115 Abshire, J. B., Bernath, P., Biraud, S. C., Blavier, J.-F. L., Boone, C., Bowman, K. P.,
 1116 Browell, E. V., Campos, T., Connor, B. J., Daube, B. C., Deutscher, N. M., Diao, M., Elkins,
 1117 J. W., Gerbig, C., Gottlieb, E., Griffith, D. W. T., Hurst, D. F., Jimenez, R., Keppel-Aleks, G.,
 1118 Kort, E. A., Macatangay, R., Machida, T., Matsueda, H., Moore, F., Morino, I., Park, S.,
 1119 Robinson, J., Roehl, C. M., Sawa, Y., Sherlock, V., Sweeney, C., Tanaka, T., Zondlo, M. A.
 1120 (2010), Calibration of the Total Carbon Column Observing Network using aircraft profile
 1121 data, *Atmos. Meas. Tech.*, 3, 1351–1362, doi:10.5194/amt-3-1351-2010, [http://www.atmos-](http://www.atmos-meas-tech.net/3/1351/2010/)
 1122 [meas-tech.net/3/1351/2010/](http://www.atmos-meas-tech.net/3/1351/2010/).

1123 Wunch, D., Toon, G. C., Blavier, J.-F. L., Washenfelder, R. A., Notholt, J., Connor, B. J., Griffith, D.
 1124 W. T., Sherlock, V., Wennberg, P. O. (2011a), The Total Carbon Column Observing Network,
 1125 *Phil. Trans. R. Soc. A*, 369, 2087–2112, doi:10.1098/rsta.2010.0240.

1126 Wunch, D., Wennberg, P. O., Toon, G. C., Connor, B. J., Fisher, B., Osterman, G. B., Frankenberg,
 1127 C., Mandrake, L., O'Dell, C., Ahonen, P., Biraud, S. C., Castano, R., Cressie, N., Crisp, D.,

1128 Deutscher, N. M., Eldering, A., Fisher, M. L., Griffith, D. W. T., Gunson, M., Heikkinen, P.,
 1129 Keppel-Aleks, G., Kyrö, E., Lindenmaier, R., Macatangay, R., Mendonca, J., Messerschmidt,
 1130 J., Miller, C. E., Morino, I., Notholt, J., Oyafuso, F. A., Rettinger, M., Robinson, J., Roehl,
 1131 C. M., Salawitch, R. J., Sherlock, V., Strong, K., Sussmann, R., Tanaka, T., Thompson, D. R.,
 1132 Uchino, O., Warneke, T., Wofsy, S. C. (2011b), A method for evaluating bias in global
 1133 measurements of CO₂ total columns from space, *Atmos. Chem. Phys.*, 11, 12317-12337.
 1134 Yoshida, Y., Ota, Y., Eguchi, N., Kikuchi, N., Nobuta, K., Tran, H., Morino, I., Yokota, T. (2011):
 1135 Retrieval algorithm for CO₂ and CH₄ column abundances from short-wavelength infrared
 1136 spectral observations by the Greenhouse gases observing satellite, *Atmos. Meas. Tech.*, 4, 717–
 1137 734, doi:10.5194/amt-4-717-2011.
 1138
 1139

11. Tables

Table 1: GHG-CCI XCO₂ and XCH₄ random and systematic uncertainty requirements for measurements over land. Abbreviations: G=Goal requirement (the maximum that needs to be achieved; better performance likely not needed as other errors (e.g., modelling errors) will dominate), B=Breakthrough requirement (“good” performance somewhere between G and T), T=Threshold requirement (the minimum that needs to be achieved for the specified application, here: global regional-scale surface flux inverse modelling). See also main text for a detailed explanation. From GHG-CCI User Requirements Document (URD, Buchwitz et al., 2011a).

Requirements for regional CO ₂ and CH ₄ source/sink determination using SCIAMACHY/ENVISAT and TANSO/GOSAT					
Parameter	Requirement type	Random error		Systematic error	Stability
		Single observation	1000 ² km ² , monthly		
XCO ₂	G	< 1 ppm	< 0.3 ppm	< 0.2 ppm (absolute)	As systematic error but per year
	B	< 3 ppm	< 1.0 ppm	< 0.3 ppm (relative)	-“-
	T	< 8 ppm	< 1.3 ppm	< 0.5 ppm (relative)	-“-
XCH ₄	G	< 9 ppb	< 3 ppb	< 1 ppb (absolute)	As systematic error but per year
	B	< 17 ppb	< 5 ppb	< 5 ppb (relative)	-“-
	T	< 34 ppb	< 11 ppb	< 10 ppb (relative)	-“-

1153

1154 **Table 2:** Overview GHG-CCI ECV Core Algorithms (ECAs). Details on each of these algorithms are
 1155 also given in the GHG-CCI ATBD (Reuter et al., 2012a) and in Buchwitz et al., 2012a. Column
 1156 “Algorithm short name” lists the GHG-CCI algorithm identifiers (names in brackets are names (also)
 1157 used in the literature (see column “References”)).

GHG-CCI ECV Core Algorithms (ECAs)				
Algorithm ID	Data product	Sensor	Algorithm short name	References
CO2_SCI_WFMD	XCO ₂	SCIAMACHY/ ENVISAT	WFMD (WFM-DOAS)	<i>Schneising et al., 2011, 2012;</i> <i>Heymann et al., 2012b</i>
CO2_SCI_BESD	XCO ₂	SCIAMACHY	BESD	<i>Reuter et al., 2010, 2011</i>
CO2_GOS_OCFP	XCO ₂	TANSO/GOSAT	OCFP (UoL-FP)	<i>Cogan et al., 2012</i>
CO2_GOS_SRFP	XCO ₂	TANSO/GOSAT	SRFP (RemoteC)	<i>Butz et al., 2011</i>
CH4_SCI_WFMD	XCH ₄	SCIAMACHY	WFMD (WFM-DOAS)	<i>Schneising et al., 2010, 2011</i>
CH4_SCI_IMAP	XCH ₄	SCIAMACHY	IMAP	<i>Frankenberg et al., 2011</i>
CH4_GOS_OCFP	XCH ₄	TANSO/GOSAT	OCFP	<i>Parker et al., 2011</i>
CH4_GOS_OCPR	XCH ₄	TANSO/GOSAT	OCPR	<i>Parker et al., 2011</i>
CH4_GOS_SRFP	XCH ₄	TANSO/GOSAT	SRFP	<i>Butz et al., 2011</i>
CH4_GOS_SRPR	XCH ₄	TANSO/GOSAT	SRPR	<i>Schepers et al., 2012</i>

1158

1159

1160 **Table 3:** Overview GHG-CCI Additional Constraints Algorithms (ACAs). (*) Note that

1161 CO2_SCI_ONPD is a new algorithm “similar” as the one described in Noël et al., 2011, which has

1162 been added in the 2nd year of GHG-CCI. Details on each of these algorithms are also given in the

1163 GHG-CCI ATBD (Reuter et al., 2012a) and in Buchwitz et al., 2012a.

GHG-CCI Additional Constraints Algorithms (ACAs)				
Algorithm ID	Data product	Sensor	Algorithm	References
CO2_AIR_NLIS	Mid/upper trop. column	AIRS	NLIS	<i>Crevoisier et al., 2004</i>
CO2_IAS_NLIS	Mid/upper trop. column	IASI	NLIS	<i>Crevoisier et al., 2009a</i>
CO2_ACE_CLRS	Upper trop. / strat. profile	ACE-FTS	CLRS	<i>Foucher et al., 2009</i>
CO2_SCI_ONPD	Stratospheric profile	SCIAMACHY	ONPD	<i>(Noël et al., 2011) (*)</i>
CH4_IAS_NLIS	Upper trop. / strat. profile	IASI	NLIS	<i>Crevoisier et al., 2009b</i>
CH4_MIP_IMK	Upper trop. / strat. profile	MIPAS	KIT/IMK MIPAS	<i>von Clarmann et al., 2009</i>
CH4_SCI_ONPD	Stratospheric profile	SCIAMACHY	ONPD	<i>Noël et al., 2011</i>

1164

1165

1166

1167

1168 **Table 4:** TCCON sites as used for the validation of the satellite-derived XCH₄ and XCO₂ Round

1169 Robin (RR) data products by the GHG-CCI validation team (from Notholt et al., 2012).

TCCON validation sites used for GHG-CCI Round Robin					
Name	ID	Latitude [deg]	Longitude [deg]	Altitude [km]	Time coverage MM/YYYY-MM/YYYY
Bialystok	BIA	53.231	23.025	0.183	03/2009 - 03/2011
Bremen	BRE	53.104	8.850	0.027	01/2009 - 12/2010
Karlsruhe	KAR	49.102	8.440	0.110	04/2010 - 05/2011
Orleans	ORL	47.965	2.113	0.132	08/2009 - 11/2010
Garmisch	GAR	47.476	11.063	0.744	05/2009 - 12/2010
ParkFalls	PAR	45.945	-90.273	0.442	06/2004 - 04/2011
Lamont	LAM	36.604	-97.486	0.320	07/2008 - 05/2011
Darwin	DAR	-12.425	130.891	0.030	08/2005 - 02/2011
Wollongong	WOL	-34.406	150.879	0.030	06/2008 - 03/2011
Lauder	LAU	-45.050	169.680	0.370	06/2004 - 06/2011

1170

1171

1172

Table 5: Estimated precision and biases of the satellite XCO₂ (top) and XCH₄ (bottom) GHG-CCI core data products retrieved with ECAs obtained from comparisons with ground-based TCCON retrievals (see Figure 3 and 4 for details). *) The exact version number for BESD is v01.00.01. Numbers in curved brackets are for SCIAMACHY methane retrievals during 2003-2005, i.e., before significant detector degradation of the methane channel: values from Buchwitz et al., 2012a, are indicated by #) and value from Schneising et al., 2012, is indicated by §). Values in square brackets for SCIAMACHY methane retrieval are from Buchwitz et al., 2012a, based on an analysis of all available retrievals (all years) and using a different assessment method. Also listed are the GHG-CCI user requirements as given the GHG-CCI User Requirements Document (URD (Buchwitz et al., 2011a), see also Table 1, e.g., for the explanation of T, B, G).

Comparison of GHG-CCI core data products (ECAs) with TCCON				
XCO ₂ [ppm]				
Algorithm	Sensor	Estimated precision single observation	Estimated relative biases	Number of satellite obs.
WFMD v2.2	SCIAMACHY	5.1	1.3	30752
BESD v1 *)	SCIAMACHY	2.3	0.7	9467
OCFP v3.0	TANSO	2.7	0.6	2830
SRFP v1.1	TANSO	2.8	0.9	2558
Required (URD):		< 8(T), 3(B), 1(G)	< 0.5(T), 0.3(B), 0.2(G)	-
XCH ₄ [ppb]				
Algorithm	Sensor	Estimated precision single observation	Estimated relative biases	Number of satellite obs.
WFMD v2.3	SCIAMACHY	82 (~30 [#])	11 (~3 [§]) [4-12 [#]]	37628
IMAP v6.0	SCIAMACHY	50 (~30 [#])	15 [4-13 [#]]	39489
OCFP v3.2	TANSO	16	8	3176
SRFP v1.1	TANSO	15	3	2558
OCPR v3.2	TANSO	13	2	7323
SRPR v1.1	TANSO	14	3	4900
Required (URD):		< 34(T), 17(B), 9(G)	< 10(T), 5(B), 3(G)	-

1186

1187 **Table 6:** Overview of the planned content of the GHG-CCI CRDP. §) see Table 2 and Table 3, *) may
 1188 end later, +) may start earlier, #) mainly high latitudes. Products: (1) mid/upper tropospheric columns,
 1189 (2) (primarily) stratospheric vertical profiles.

Planned content of the GHG-CCI Climate Research Data Package (CRDP)				
Data products generated with ECV Core Algorithms (ECAs)				
Product ID	Product (Level 2, mixing ratios)	Algorithm §)	Coverage	Comment
XCO2_SCIA	XCO ₂	BESD	Global, land, 2003-2010 ^{*)}	-
XCO2_GOSAT	XCO ₂	OCFP and SRFP	Global, mid 2009-2010 ^{*)}	2 alternative products
XCO2_EMMA	XCO ₂	EMMA	Global, mid 2009-2010 ^{*)}	Merged SCIA and GOSAT
XCH4_SCIA	XCH ₄	IMAP and WFMD	Global, 2003-2010 ^{*)}	2 alternative products
XCH4_GOSAT	XCH ₄	SRFP and OCPR	Global, mid 2009-2010 ^{*)}	2 alternative products
Data products generated with Additional Constraints Algorithms (ACAs)				
Product ID	Product (Level 2, mixing ratios)	Algorithm §)	Coverage	Comment
CO2_AIRS	CO ₂ (1)	NLIS	Tropics, 2003-2007	-
CO2_IASI	CO ₂ (1)	NLIS	Tropics, 2007-2010 ^{*)}	-
CH4_IASI	CH ₄ (1)	NLIS	Tropics, 2007-2010 ^{*)}	-
CH4_SCIA_OCC	CH ₄ (2)	ONPD	NH mid/high lat., 2003-2010 ^{*)}	-
CO2_SCI_OCC	CO ₂ (2)	ONPD	NH mid/high lat., 2003-2010 ^{*)}	-
CH4_MIPAS	CH ₄ (2)	KIT/IMK MIPAS	Global, 2005 ^{+) - 2010^{*)}}	-
CO2_ACEFTS	CO ₂ (2)	CLRS	Global ^{#)} , 2004-2010 ^{*)}	-

1190

1191

1192

1193 **12. Figures**

1194

1195 **Figure 1:** Top: Northern hemispheric monthly mean XCO₂ time series retrieved from

1196 SCIAMACHY/ENVISAT (algorithms: WFMD and BESD) and TANSO/GOSAT (algorithms: SRFP

1197 and OCFP) satellite data. Shown are monthly mean values for the 0°-60°N latitude range. Clearly

1198 visible is the CO₂ increase primarily caused by the burning of fossil fuels and the seasonal cycle

1199 primarily caused by uptake and release of CO₂ by the terrestrial biosphere. Bottom: As top panel but

1200 for XCH₄ (algorithms: SCIAMACHY: WFMD and IMAP, TANSO: SRFP, SRPR, OCFP, OCPR).

1201 The seasonal cycle of methane is primarily due to wetland emissions, which are largest in summer /

1202 early autumn, when soils are warm and humid. Also clearly visible is the not yet well understood

1203 recent methane increase. For a color version of this figure please have a look at the on-line version of

1204 this publication.

Figure 2: Global XCO₂ maps from SCIAMACHY (left) and CarbonTracker (right) for two seasons (April-June, top, and July-September, bottom) and two years (2003 and 2009). The CarbonTracker model data have been sampled according to the SCIAMACHY measurements and the SCIAMACHY averaging kernels have been applied to CarbonTracker. Figure adapted from Heymann et al., 2012b. For a color version of this figure please have a look at the on-line version of this publication.

1217

Satellite - TCCON differences: XCO₂

1218

1219

1220

1221 **Figure 3:** Comparison of the GHG-CCI core ECV XCO₂ data products from
1222 SCIAMACHY/ENVISAT (top half, i.e., first 3 panels) and TANSO/GOSAT (bottom half) with
1223 TCCON ground-based observations (see Table 4 for details on the TCCON sites). Shown are the mean
1224 difference (“Mean” in ppm) with respect to TCCON (left), the standard deviation of the difference
1225 (right), and the number of co-locations (middle). A 500 km / 2 hour spatio-temporal co-location
1226 criterion has been used to compute the satellite – TCCON differences. The numerical values listed are:
1227 Left: “StdDev” is the standard deviation of the mean differences as obtained at the TCCON sites, i.e.,
1228 a measure of the station-to-station bias, and can be interpreted as relative accuracy (relative bias) of
1229 the satellite retrievals. “N” is the number of satellite data used for comparison (only those data points
1230 are shown where at least 10 satellite observations are available for a given site). Right: “Mean” is the
1231 mean value of the standard deviations show by the symbols and is a measure of the achieved overall
1232 precision. Note that the number of co-locations is significantly different for the different TCCON sites,
1233 e.g., due to clouds. For a color version of this figure please have a look at the on-line version of this
1234 publication.

1235

Satellite - TCCON differences: XCH₄

Figure 4: As Fig. 3 but for the GHG-CCI XCH₄ data products.

1243

1244

1245

Figure 5: Maps of monthly mean XCO₂ at 10°x10° resolution as obtained using different GHG-CCI retrieval algorithms: WFMD and BESD for SCIAMACHY, OCFP and SRFP for TANSO and SCIAMACHY and TANSO merged using EMMA for September 2009 (left) and May 2012 (right).

1247

1248

For a color version of this figure please have a look at the on-line version of this publication.

1249

1250

1251

1252

1253

1254 **Figure 6:** Comparison matrix of monthly XCO₂ maps for September 2009 (top (a)) and May 2010
1255 (bottom (b)) generated using several individual satellite retrieval algorithms: BESD and WFMD for
1256 SCIAMACHY and SRFP, ACOS, OCFP, PPDF, NIES for TANSO. The EMMA data product has
1257 been generated from the ensemble of the individual SCIAMACHY and TANSO XCO₂ data products
1258 (see main text for details). Also shown is XCO₂ from TCCON and NOAA's CarbonTracker (CT,
1259 v2011). The diagonal elements show the monthly XCO₂ maps (using color bar "mean"). The above
1260 diagonal elements show the XCO₂ differences for all combinations (color bar "difference"). The below
1261 diagonal elements show the numerical values of the Root Mean Square Difference (RMSD) as well as
1262 color coded smileys of the RMSD (green: RMSD < 1.2 ppm, red: RMSD > 2.4 ppm, otherwise
1263 yellow). For a color version of this figure please have a look at the on-line version of this publication.

1264

Figure 7: Pie charts showing the agreement (left) and disagreement (right) with the EMMA median obtained using the listed satellite XCO₂ data products. The figure has been obtained using the EMMA Level 3 data product (10°x10°, monthly = 1 voxel). For each voxel the mean XCO₂ value for each algorithm has been computed and the median using all algorithms. The “Agreement with the Median” (left) has been computed as follows: For algorithm *i* the number of voxels which agree with the median within 0.2 ppm have been counted (= N_i). 100% corresponds to the sum of these numbers ($N = \sum_i N_i$). The percentages shown are $N_i/N \times 100\%$. The percentages of “Potential Outliers” (right) have been calculated using the same method except that all voxels have been counted where the differences to the median are larger than 2 ppm. As can be seen from the left figure, the data product which agrees best with the median is the ACOS product (v2.9, 21% agreement) followed by the similar OCFP algorithm (19% agreement). The largest number of potential outliers have the data products generated with the two very fast algorithms WFMD (32%) and PPDF (16%). For a color version of this figure please have a look at the on-line version of this publication.

1283

1284

1285

1286

1287

1288

1289

1290

1291

1292

1293

Figure 8: Comparison of the XCO₂ seasonal cycle amplitude (peak-to-peak) of the individual XCO₂ algorithms and EMMA with TCCON (left) and CarbonTracker (v2011) (right). The figure has been adapted from Reuter et al., 2013, where results for all investigated XCO₂ data products are shown, i.e., including WFMD and PPDF, not shown here as their error bars do not indicate good enough agreement with TCCON. As can be seen, all XCO₂ satellite data suggest that the amplitude of the CO₂ seasonal cycle is underestimated by CarbonTracker by approximately 1.5+/-0.5 ppm peak-to-peak. For a color version of this figure please have a look at the on-line version of this publication.

1294

1295

1296

1297

1298

1299

1300

1301

1302

Figure 9: Comparison of two SCIAMACHY XCH₄ data products retrieved using WFMD (top) and IMAP (middle) for August 2005. Global maps of the retrieved XCH₄ are shown on the left and the number of retrievals per 5°x5° grid cell on the right. The WFMD-IMAP difference is shown in the bottom row. Listed in the bottom left are the following parameters: d: mean difference (-2.12 ppb), s: standard deviation of the difference (18.53 ppb), r: linear correlation coefficient (0.75). For a color version of this figure please have a look at the on-line version of this publication.

1303

1304

1305 **Figure 10:** As Fig. 9 but for July 2009.

1306

1307

1308

1309

1310

1311 **Figure 11:** Comparison of the two GHG-CCI TANSO XCH₄ PR data products retrieved using the
1312 OCPR and SRPR retrieval algorithms. Left: Percentage XCH₄ difference OCPR-SRPR for July 2009.
1313 Right: Scatter plot of 6751 co-located OCPR versus SRPR retrievals at TCCON sites. The standard
1314 deviation of the difference is 10 ppb (1-sigma) and the linear correlation coefficient is 0.91. For a color
1315 version of this figure please have a look at the on-line version of this publication.

1316