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Assessing 5 years of GOSAT Proxy XCH$_4$ data and associated uncertainties

R. J. Parker$^{1,2}$, H. Boesch$^{1,2}$, K. Byckling$^1$, A. J. Webb$^1$, P. I. Palmer$^{3,4}$, L. Feng$^{3,4}$, P. Bergamaschi$^5$, F. Chevallier$^6$, J. Notholt$^7$, N. Deutscher$^{2,11}$, T. Warneke$^7$, F. Hase$^8$, R. Sussmann$^8$, S. Kawakami$^9$, R. Kivi$^{10}$, D. W. T. Griffith$^{11}$, and V. Velazco$^{11}$

$^1$Earth Observation Science, Department of Physics and Astronomy, University of Leicester, Leicester, UK
$^2$National Centre for Earth Observation, Department of Physics and Astronomy, University of Leicester, Leicester, UK
$^3$School of GeoSciences, University of Edinburgh, Edinburgh, UK
$^4$National Centre for Earth Observation, School of GeoSciences, University of Edinburgh, Edinburgh, UK
$^5$European Commission Joint Research Centre, Institute for Environment and Sustainability, Ispra, Italy
$^6$Lab. des Sciences du Climat et de l’Environnement, CNRS, Gif-sur-Yvette, France
$^7$Institute of Environmental Physics, University of Bremen, Bremen, Germany
$^8$Karlsruhe Institut für Technologie, Karlsruhe, Germany
$^9$Japan Aerospace Exploration Agency (JAXA), Tsukuba, Japan
$^{10}$Finnish Meteorological Institute, Arctic Research, Saodanykylä, Finland
$^{11}$School of Chemistry, University of Wollongong, Wollongong, Australia

Correspondence to: R. J. Parker (rjp23@le.ac.uk)

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Abstract. We present 5 years of GOSAT XCH$_4$ retrieved using the “proxy” approach. The Proxy XCH$_4$ data are validated against ground-based TCCON observations and are found to be of high quality with a small bias of 4.8 ppb ($\sim 0.27\%$) and a single-sounding precision of 13.4 ppb ($\sim 0.74\%$). The station-to-station bias (a measure of the relative accuracy) is found to be 4.2 ppb. For the first time the XCH$_4$ / XCO$_2$ ratio component of the Proxy retrieval is validated (bias of 0.014 ppb ppm$^{-1}$ ($\sim 0.30\%$), single-sounding precision of 0.033 ppb ppm$^{-1}$ ($\sim 0.72\%$)).

The uncertainty relating to the model XCO$_2$ component of the Proxy XCH$_4$ is assessed through the use of an ensemble of XCO$_2$ models. While each individual XCO$_2$ model is found to agree well with the TCCON validation data ($r = 0.94\text{--}0.97$), it is not possible to select one model as the best from our comparisons. The median XCO$_2$ value of the ensemble has a smaller scatter against TCCON (a standard deviation of 0.92 ppm) than any of the individual models whilst maintaining a small bias (0.15 ppm). This model median XCO$_2$ is used to calculate the Proxy XCH$_4$ with the maximum deviation of the ensemble from the median used as an estimate of the uncertainty.

We compare this uncertainty to the a posteriori retrieval error (which is assumed to reduce with $\sqrt{N}$) and find typically that the model XCO$_2$ uncertainty becomes significant during summer months when the a posteriori error is at its lowest due to the increase in signal related to increased summertime reflected sunlight.

We assess the significance of these model and retrieval uncertainties on flux inversion by comparing the GOSAT XCH$_4$ against modelled XCH$_4$ from TM5-4DVAR constrained by NOAA surface observations (MACC reanalysis scenario S1-NOAA). We find that for the majority of regions the differences are much larger than the estimated uncertainties. Our findings show that useful information will be provided to the inversions for the majority of regions in addition to that already provided by the assimilated surface measurements.

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1 Introduction

Atmospheric methane (CH$_4$) contributes significantly to the Earth’s radiative forcing budget (Myhre et al., 2013), making it the second most important anthropogenic greenhouse gas after carbon dioxide (CO$_2$). The major sources of atmospheric methane include wetland emission, rice production, enteric fermentation (cattle), termites, biomass burning, fossil fuel production, and waste (Bousquet et al., 2006). There remains, however, a large degree of uncertainty on the magnitude of these individual sources (Kirschke et al., 2013).

The lifetime of CH$_4$ in the atmosphere is mainly controlled by its reaction with the hydroxyl free radical (OH), resulting in an atmospheric lifetime of approximately 9 years (Prather et al., 2012). Given its long atmospheric lifetime, there is a need for long-term global measurements to fully understand how the atmospheric distribution of CH$_4$ is evolving with time. Indeed, recent unexpected variability in the atmospheric growth rate of methane has emphasised gaps in our current understanding (Rigby et al., 2008; Dlugokencky et al., 2009; Nisbet et al., 2014).

In order to begin to understand the spatio-temporal distribution of atmospheric methane, regular global satellite observations of CH$_4$ can be coupled with highly precise but geographically sparse surface concentration data. Through the combination of both data sources, the large uncertainties related to the upscaling of surface concentration data can be minimised whilst also obtaining information in remote regions where surface measurements are not available.

Various studies have demonstrated the utility of such space-borne measurements in determining the regional surface fluxes of methane using data from the SCIAMACHY (Bergamaschi et al., 2007, 2009, 2013; Houweling et al., 2014) and Greenhouse gases Observing SATellite (GOSAT) (Fraser et al., 2013; Cressot et al., 2014; Monteil et al., 2013; Alexe et al., 2015) instruments.

The SCIAMACHY instrument operated onboard ENVISAT and provided a 9-year record (2003–2012) of global methane total column observations (Schneising et al., 2011; Frankenberg et al., 2011). The continuation of this time series of space-based observations was ensured by the launch of the first dedicated greenhouse gas measuring satellite, the Japanese GOSAT, in 2009 (Yokota et al., 2009). GOSAT provides global coverage with a 3-day repeat cycle and was designed with the intention of characterising continental-scale sources and sinks.

In a previous work (Parker et al., 2011) we presented the first year of our global short-wave infrared (SWIR) measurements of the dry-air column-averaged mole fraction of CH$_4$ (XCH$_4$) from the GOSAT mission using the “proxy” retrieval approach. This data product has subsequently been developed (Buchwitz et al., 2013) and validated (Dils et al., 2014) as part of the ESA Climate Change Initiative Greenhouse Gas project and we now report an assessment of the full 5-year data set for version 5.0 of the University of Leicester GOSAT Proxy XCH$_4$ data product.

This work is motivated by the desire to better understand the uncertainty characteristics of the Proxy XCH$_4$ data for use within flux inversion systems, especially relating to uncertainties introduced by the model XCO$_2$.

In Sect. 2 we describe the retrieval approach, including details of the updates since the original version of the University of Leicester GOSAT Proxy XCH$_4$ data (Parker et al., 2011). In Sect. 3 we compare both the Proxy XCH$_4$ and the XCH$_4$ / XCO$_2$ ratio against the ground-based validation data. In Sect. 4 we assess the CO$_2$ model component of the Proxy XCH$_4$ for the first time, with Sect. 5 then discussing the associated uncertainty of the final Proxy XCH$_4$ product and its utility in constraining surface fluxes within an inversion framework. Finally, we conclude the paper in Sect. 6 and provide recommendations for data users.

2 University of Leicester GOSAT Proxy XCH$_4$ retrieval updates

The University of Leicester GOSAT Proxy XCH$_4$ retrieval utilises the Orbiting Carbon Observatory (OCO) “full physics” retrieval algorithm, developed for the original NASA OCO mission to retrieve XCO$_2$ (dry-air column-averaged mole fraction of CO$_2$) from a simultaneous fit of SWIR O$_2$ and CO$_2$ bands and has subsequently been modified to operate on GOSAT spectral data.

Full details of the OCO retrieval algorithm can be found in O’Dell et al. (2012). In short, the retrieval algorithm utilises an iterative retrieval scheme based on Bayesian optimal estimation to estimate a set of atmospheric, surface, and instrument parameters from the measured spectral radiances, referred to as the state vector. The state vector of our retrieval consists of 20-level profiles for CH$_4$ and CO$_2$ volume mixing ratios (vmr), profile scaling factors for H$_2$O vmr, and temperature, surface albedo, and spectral dispersion.

Rather than perform the “full physics” retrieval as typically used for CO$_2$ (Connor et al., 2008; Boesch et al., 2011), an alternative approach is possible for CH$_4$, the so-called “proxy” method. First used for the retrieval of XCH$_4$ from SCIAMACHY (Frankenberg et al., 2006), this approach uses the fact that there exists CO$_2$ and CH$_4$ spectral signatures located close together at around 1.6 µm and hence the majority of atmospheric scattering and instrument effects will be similar between the two bands. The ratio of the retrieved XCH$_4$ / XCO$_2$ should cancel modifications to the length of the light path that are experienced due to scattering (Butz et al., 2010), with the CO$_2$ effectively acting as a “proxy” for the unknown light-path enhancements. As CO$_2$ is known to vary much less than CH$_4$, the final XCH$_4$ product can be obtained by multiplying this XCH$_4$ / XCO$_2$ ratio by a model CO$_2$ value, typically taken from a global chemistry transport model (Eq. 1).
The “proxy” retrieval approach has various advantages over the full physics approach (Schepers et al., 2012). Because there is no reliance on an explicit a priori knowledge of the aerosol distribution, the proxy approach is more robust in the presence of aerosols and also far less sensitive to instrumental issues or inconsistent radiometric calibration between the spectral bands than is the case for the full physics approach. Additionally, as moderate scattering from aerosols will be cancelled out and still result in an accurate retrieval of XCH$_4$, the number of successful soundings for the proxy approach is typically much higher than for the full physics approach which requires far stricter post-filtering. This leads not only to more soundings in general but also to more soundings over regions where very little full physics data may be available, such as in the tropics.

The main disadvantage with the proxy approach is that it is reliant on an accurate, unbiased model XCO$_2$ data set to convert the XCH$_4$ / XCO$_2$ ratio back into an XCH$_4$ quantity; otherwise errors relating to the model XCO$_2$ may be folded into the final XCH$_4$ result. Here we present assessments of the different uncertainties to determine the importance of this aspect of the Proxy XCH$_4$ data.

We process the latest versions of the GOSAT Level 1B files (version 161.160) acquired directly from the NIES Large Volume Data Server and apply the recommended radiometric calibration and radiometric degradation correction as per Kuze et al. (2014).

For the spectroscopic inputs we use v4.2.0 of the OCO line lists with CH$_4$ taken from the Total Carbon Column Observing Network (TCCON) line lists (version “20120409”). The a priori pressure, temperature, and water vapour is taken from the ECMWF ERA-Interim data (Dee et al., 2011). For the CO$_2$ a priori we use the MACC-II CO$_2$ inversion (v13r1) and for the CH$_4$ we use the MACC-II CH$_4$ inversion (v10-S1NOAA, using 2012 data for 2013) but here we adjust the stratospheric methane using a specialised full chemistry run (run ID 563) of the TOMCAT stratospheric chemistry model from the University of Leeds (Chipperfield, 1999). This TOMCAT model run has been validated against ACE-FTS observations and was found to provide a more accurate representation of the stratosphere.

The spectral noise is estimated from the standard deviation of the out-of-band signal. Spectra over ocean or with a signal-to-noise ratio (SNR) below 50 are removed. Cloud-contaminated scenes are removed by the comparison of a clear-sky surface pressure retrieval from the O$_2$ A-band to the ECMWF surface pressure for the relevant measurement time and location. A scene is determined to be cloudy when the retrieved surface pressure differs by more than 30 hPa from the estimated ECMWF surface pressure. This relatively loose threshold is allowed as the proxy retrieval approach remains relatively robust in the presence of near-surface clouds. The average difference between our retrieved surface pressure and ECMWF after filtering for cloud is approximately 3 hPa with a standard deviation of below 10 hPa, with the offset from 0 hPa being attributed to spectroscopic uncertainties in the O$_2$ cross-sections. The Proxy XCH$_4$ retrieval is performed for all scenes that are deemed to be sufficiently cloud free.

After filtering for signal-to-noise, cloud, and data quality we are left with 1 032 760 XCH$_4$ retrievals over land between April 2009 and December 2013. Figure 1 shows global maps of the Proxy XCH$_4$ for each season and compares it to the MACC-II model XCH$_4$ data. Both model and observation show the XCH$_4$ variability in time and space, in particular with the large emissions of methane from wetland and rice cultivation over India and S.E. Asia.

3 Validation of the Proxy XCH$_4$ and XCH$_4$/XCO$_2$ ratio

This section presents the validation of the University of Leicester GOSAT Proxy XCH$_4$ v5.0 data through comparison to observations from the ground-based TCCON. In addition, for the first time the XCH$_4$ / XCO$_2$ ratio itself, the core component of the Proxy XCH$_4$ data, is validated against the corresponding TCCON data.

TCCON is a global network of ground-based high-resolution Fourier transform spectrometers recording direct solar spectra in the near-infrared spectral region (Wunch et al., 2011a). The TCCON data are calibrated to World Meteorological Organization (WMO) standards by calibration against aircraft measurements (Wunch et al., 2010). Although it should be noted that this aircraft calibration does not measure the whole column, the TCCON data are the standard against which current satellite observations of greenhouse gases are validated (Cogan et al., 2012; Wunch et al., 2011b; Dils et al., 2014).

To date, all previous validation of satellite greenhouse gas observations against TCCON has used TCCON data that were affected by instrumental biases relating to a laser sampling error which resulted in an XCO$_2$ error of approximately 0.26% (1 ppm) (Messerschmidt et al., 2010). Although the corresponding XCH$_4$ error was not quantified, it is expected that it would be of similar magnitude (i.e. 1 part in 400). The latest, recently released, version of the TCCON data (GGG2014) incorporates a correction for the laser sampling errors and any remaining bias is expected to be small.

Figure 2 shows the GGG2014 TCCON XCH$_4$ data and the Proxy XCH$_4$ plotted as time series for each TCCON site. The mean GOSAT−TCCON difference, the standard deviation of the GOSAT−TCCON difference, the correlation coefficient, and the number of soundings are all provided for each site.
Figure 1. Seasonal global maps of the University of Leicester GOSAT Proxy $\text{XCH}_4$ (top) and the MACC-II (bottom) model $\text{XCH}_4$ data (v10-S1NOAA). Both model and observation show the $\text{XCH}_4$ variability in time and space, in particular with the large emissions of methane from wetland and rice cultivation over India and S.E. Asia. Note that GOSAT changed their pointing pattern in August 2010 from five across-track points to three across-track points, resulting in a change in spatial coverage.

Figure 3 (top) shows the correlation between the GGG2014 TCCON $\text{XCH}_4$ data and the Proxy $\text{XCH}_4$ values within $\pm 5^{\circ}$ of each TCCON site and a temporal coincidence of $\pm 2$ h. It should also be noted that for all TCCON comparisons, the difference inherent in the data due to using different a priori has been compensated for (as discussed in Rodgers (2000), by replacing the a priori used in the GOSAT retrievals with the TCCON a priori after the retrieval has been performed) which typically increases the GOSAT $\text{XCH}_4$ data by an average of between 0 and 5 ppb with the larger effect seen at more northerly TCCON stations. We use all TCCON sites where version GGG2014 has been processed at the time.
of writing that contain data during the GOSAT time period (2009–2014). This results in 11 TCCON stations ranging from Sodankylä, Finland, at 67.4° N to Lauder, New Zealand, at 45.0° S. The correlation between the GOSAT and TCCON data is reasonable/good across all sites, ranging from 0.54 at Karlsruhe to 0.79 at Lauder with an overall correlation coefficient of 0.87 between 22,619 points. The overall bias is found to be 4.8 ppb with an overall single measurement precision of 13.4 ppb (ranging from 8.3 ppb at Darwin to 14.9 ppb at Garmisch). The station-to-station bias, which is an indication of the relative accuracy, is calculated as the standard deviation of the individual site biases and is found to be just 4.2 ppb.

In addition to the validation of the Proxy XCH<sub>4</sub> data, we also present for the first time the validation of the XCH<sub>4</sub> / XCO<sub>2</sub> ratio. This ratio is the quantity directly retrieved from the satellite measurement, is independent of any model XCO<sub>2</sub>, and has recently itself been used directly within a flux inversion study (Fraser et al., 2014). The correlation coefficient across all stations is found to be 0.88 (ranging from 0.6 at Wollongong to 0.88 at Sodankylä) with a mean bias of 0.014 ppb ppm<sup>-1</sup> and a single-sounding precision of 0.033 ppb ppm<sup>-1</sup> (ranging from 0.20 ppb ppm<sup>-1</sup> at Darwin to 0.037 ppb ppm<sup>-1</sup> at Garmisch). The statistics for the XCH<sub>4</sub> / XCO<sub>2</sub> ratio are therefore comparable to those of the Proxy XCH<sub>4</sub> itself, suggesting that the majority of the variation is from the satellite retrieval itself and not introduced by the model XCO<sub>2</sub>. The next section investigates this aspect in more detail.

4 Assessing the CO<sub>2</sub> model ensemble component

In Sect. 3 the final Proxy XCH<sub>4</sub> and the XCH<sub>4</sub> / XCO<sub>2</sub> component were both validated against the TCCON data. In this section we validate the remaining component of the proxy product from Eq. (1), namely the model XCO<sub>2</sub>.

As discussed in Sect. 2, this update to the University of Leicester GOSAT Proxy XCH<sub>4</sub> data uses an ensemble of model XCO<sub>2</sub> data to act as the model XCO<sub>2</sub> component. We utilise the XCO<sub>2</sub> from three state-of-the-art global transport models which all assimilate surface in situ measurements; GEOS-Chem (University of Edinburgh – Feng et al., 2011, v1.50), MACC-II (Chevallier et al., 2010, v14r1) and CarbonTracker (NOAA – Peters et al., 2007, vCT2013B). These model runs have assimilated similar surface measurements but not necessarily from all of the same data sets or the same locations. The models also have different spatial resolutions and different temporal coverage (GEOS-Chem: 2009–2011, 5° × 4°; CarbonTracker: 2009–2012, 3° × 2°; MACC-II: 2009–2012, 3.75° × 1.89°). Where the model does not cover the full GOSAT time period studied here, the data from the previous year are used and adjusted by the NOAA annual growth rate.

The main concern with using modelled XCO<sub>2</sub> data for the proxy method is that the additional uncertainty added to the final proxy data product is difficult to determine. Where the model XCO<sub>2</sub> data are constrained by surface data there can be a high degree of confidence that the model data are close to representing the true value of CO<sub>2</sub>; however, it is away from such regions where there is a possibility of adding additional biases into the Proxy XCH<sub>4</sub> data. The TCCON stations are mostly in regions that are also well constrained by surface in situ measurements and hence the model CO<sub>2</sub> data should be well constrained, at least at the surface level, and it is therefore expected to reasonably reproduce the TCCON column data. Figure 4 confirms that this is the case. As the model XCO<sub>2</sub> is used as a component in the proxy retrievals, the models are treated as “pseudo-measurements” and validated in the same way as the satellite data in order to maintain consistency with the satellite validation. The model XCO<sub>2</sub> data sampled at each GOSAT measurement point within ± 2° of each TCCON station are found to agree well with the...
Figure 3. Correlation plot of the Proxy XCH$_4$ (top) and the XCH$_4$/XCO$_2$ ratio (bottom) data against TCCON ground-based FTS data at 11 TCCON sites. The overall bias, standard deviation (single-sounding precision), correlation coefficient, and total number of soundings are provided. Note that the Lauder TCCON station upgraded the instrument from a Bruker 120 to a Bruker 125 in February 2010 and these two data sets are displayed separately.

Figure 4. Correlation plot of the model XCO$_2$ data for GEOS-Chem, MACC-II, CarbonTracker, and the ensemble median against TCCON ground-based FTS data at 11 TCCON sites. The overall bias, standard deviation (single-measurement precision), correlation coefficient, and total number of soundings are provided separately.
TCCON data, with the correlation coefficients ranging from 0.94 (GEOS-Chem) to 0.97 (MACC-II and CarbonTracker). Similarly the precision and bias to TCCON are both found to be small (ranging from 0.97 to 1.3 and 0.07 to 0.27 ppm respectively). The relative accuracies (the standard deviation of the individual site biases) are similar at around 0.5 ppm, with CarbonTracker and GEOS-Chem performing slightly better than MACC-II. Another metric to assess the models is how often they provide the median value of the ensemble. CarbonTracker (41%) and MACC-II (36%) tend to provide the median value more often than GEOS-Chem (22%) but this can vary per site with the contribution from MACC-II as low as 27% at Darwin (and CarbonTracker at 60%) and conversely as high as 44% at Wollongong (with CarbonTracker only 21%). This provides further indication that no one model can be determined to be the “best”.

For a more detailed analysis of the performance of the different XCO$_2$ models please see Table A1 in Appendix A. In short, none of the models are found to consistently be superior over the other models. GEOS-Chem typically has the highest scatter against TCCON but also has the smallest bias at 5 out of 12 of the sites. MACC-II has the smallest bias at seven sites but the highest bias at four of the sites. CarbonTracker has the highest bias at seven of the sites but also has the smallest scatter at eight of the sites. Whilst the absolute bias in the calculated median XCO$_2$ is typically not quite as small as the best of the individual models, the scatter in the median is better than (or the same as) the best scatter from any of the individual models at every site except Lauder_120 (where the time series is the shortest) and even there it is only worse than the best model by less than 0.1 ppm.

The above has demonstrated that it is not a simple decision to determine which model most accurately represents the true atmosphere, even in locations where all of the models have been constrained by (often the same) surface measurements and high-quality validation data are available. In more remote regions where we neither have validation data nor surface measurements to constrain the models, this inconsistency between the models becomes more pronounced. It is this uncertainty in model XCO$_2$ in regions away from the available validation data that we attempt to address through the use of the XCO$_2$ model ensemble. Each of the three XCO$_2$ models are sampled at every GOSAT time and location and convolved with the scene-specific GOSAT averaging kernels. The median value of the three model values is used as the model XCO$_2$ in calculating the final Proxy XCH$_4$. However, we also define the uncertainty on this median XCO$_2$ as the maximum of the absolute differences of each individual model to the median value.

We have already demonstrated that the models all well reproduce the validation data at TCCON sites without any one model identified as being better than the others from our comparisons. Where the models all agree well with each other away from the validation sites, the assumption is that the models are accurately representing the true atmosphere. Where the models disagree with each other, we do not know which model is correct in the absence of further validation data and in some cases the discrepancy between models can be very large (i.e. > 4 ppm). In such cases where no validation is possible, the best estimate of the uncertainty in the model XCO$_2$ data is obtained by examining the difference of the model data around the median value. Figure 5 shows global maps of this estimated model uncertainty for each season. There are clear spatial/temporal patterns in the distribution of this model uncertainty. During March–May (boreal “spring”), there is a large uncertainty (> 2 ppm) over India and the African regions typically associated with biomass burning. There is also a moderate level of uncertainty (> 1 ppm) over Europe, South America, and for the latter years over North America and Australia. For the summer months (June–August) it is the Eurasian region, extending from the Ural mountains eastwards through Siberia and northern China, where the model uncertainty is largest at over 2 ppm. This is to be expected as in the Northern Hemisphere it is the period of greatest photosynthetic activity and the model sensitivity to the underlying mechanisms is likely to be largest. During boreal autumn (September–November), the uncertainty in the Northern Hemisphere is vastly reduced again, with India being the major region of uncertainty along with South America and regions of biomass burning in Africa. Winter is similar to autumn, with all three models in very good agreement with each other in the Northern Hemisphere, with only S.E. Asia showing a moderate level of uncertainty. In the Southern Hemisphere, again South America and southern Africa show moderate uncertainty which appears to be linked to emissions from biomass burning.

This section has shown that the estimated uncertainty of the model XCO$_2$ can vary greatly in time and space. When considering the implication of this uncertainty on flux inversions of the Proxy XCH$_4$ data, the relative importance of the different uncertainties must be considered. The following section investigates the distribution of the model XCO$_2$ uncertainty and judges its relative importance against the a posteriori error from the retrieval itself. Finally, both of these uncertainties are assessed against the difference to modelled XCH$_4$ already constrained by surface observations to determine the utility of the satellite data despite the presence of these uncertainties.

5 Assessing the relative uncertainties

In order to assess the importance of the uncertainty of the model XCO$_2$, we bin the three model fields into $4^\circ \times 5^\circ$ grid boxes over 8-day time steps and calculate the maximum difference of the three-model ensemble from the median value to use as an estimate of the uncertainty in the model values. We convert this uncertainty in model XCO$_2$ into an uncertainty in XCH$_4$ by multiplying each point by its respective retrieved XCH$_4$ / XCO$_2$ amount. We also calculate the av-
Figure 5. Seasonal maps of the model difference, defined as the maximum absolute difference of the three-model ensemble from the median. All individual soundings have been averaged into $2^\circ \times 2^\circ$ grid boxes over each season. The largest uncertainties occur in regions where the CO$_2$ variability is expected to be highest and the models are unconstrained by surface measurements.

Figure 6. The Transcom regions over which the $4^\circ \times 5^\circ$ gridded data are then averaged in Fig. 7.

average a posteriori error for the same data. Unlike the more systematic XCO$_2$ model uncertainty, the a posteriori error should be close to random and hence reduce approximately with the square root of the number of soundings being averaged. If the error does not reduce as much, the model XCO$_2$ component would then contribute even less to the total, leading to this assumption being a “worst case” scenario for the effect of the model XCO$_2$ uncertainty. These $4^\circ \times 5^\circ$ grid boxes are then themselves averaged over the Transcom regions (Gurney et al., 2002) as defined in Fig. 6.

In Fig. 7, the red line shows the mean of the Proxy XCH$_4$ random (a posteriori) error from each $4^\circ \times 5^\circ$ box averaged over each Transcom region with the green line representing the estimated uncertainty related to the model XCO$_2$. The majority of regions exhibit a similar trend over time. The a posteriori error peaks in the winter months when the SNR of the measurement is at its lowest and is at a minimum during the summer months when the SNR is at a maximum. This seasonal effect is more pronounced at higher latitudes which experience a greater degree of variability of sunlight throughout the year. Conversely, the XCO$_2$ model uncertainty follows biospheric activity with the uncertainty largest during the summer months when the XCO$_2$ variability is at a maximum and reduces to a minimum in the winter months when biospheric activity is lower. This leads to the situation where the a posteriori error dominates the model uncertainty in winter months but during summer months the model uncertainty can be comparable to, or even exceed, the a posteriori error. Taking the North America Temperate region as an example, during winter the a posteriori error can reach up to 8 ppb with the error from the model XCO$_2$ significantly lower with values less than 2 ppb. In contrast, during the summer months, the a posteriori error reduces to around 5 ppb but the error for the model XCO$_2$ increases to 5 ppb, meaning that both become significant components of the overall uncertainty.
We have shown that the uncertainty related to the XCO$_2$ model can, particularly in the Northern Hemisphere during summer months, be of comparable magnitude to the a posteriori retrieval error. However, that in itself does not preclude the data from adding useful information to a CH$_4$ flux inversion.

The MACC-II model XCH$_4$ (v10-S1NOAA) data have assimilated NOAA surface measurements at background sites and hence are well constrained in the remote atmosphere (Bergamaschi et al., 2013). Here we calculate the difference between the MACC XCH$_4$ model field and the GOSAT Proxy XCH$_4$ data for each GOSAT measurement (referred to from here as ΔXCH$_4$). We then aggregate these differences in the same way as the model XCO$_2$ uncertainties. Note that the MACC XCH$_4$ model data are currently only available until the end of 2012. As some inversion systems will perform a simple (e.g., latitudinal) bias correction, the calculated retrieval a posteriori and model XCO$_2$ uncertainties can potentially be much lower than the ΔXCH$_4$ value but still not provide information to the inversion. For this reason, it is also important to consider both the mean (μΔXCH$_4$) and the standard deviation (σΔXCH$_4$) of the ΔXCH$_4$. To determine whether the GOSAT data are capable of providing information to the inversion, we compare the a posteriori and model XCO$_2$ uncertainties to the μΔXCH$_4$ and σΔXCH$_4$ values as shown in Fig. 7, with the seasonal averages for all of these values presented in Table A2.

It should be noted here that the absolute values are not necessarily quantitatively comparable when taking into account how an inversion system will use the two different quantities. The a posteriori error of the retrieved XCH$_4$ is an indication of the weighting that the inversion will give to an observation over the a priori, with a smaller value indicating that the inversion will “trust” the observation more. The ΔXCH$_4$ is an indication of how much the inversion needs to adjust the fluxes in order to match the observation. However, if the estimated uncertainties are significantly less than the μΔXCH$_4$ and σΔXCH$_4$ values it is expected that the observations should provide value to the inversion. It should also be noted that this bias term (μΔXCH$_4$) may also reflect systematic biases in the XCH$_4$ model due to, for example, errors in the vertical model profile whilst the sigma term (σΔXCH$_4$) may also relate to subgrid-scale variations which are unresolved at the model resolution.

For the North American Boreal region, both the μΔXCH$_4$ and σΔXCH$_4$ values are very similar in terms of phase and magnitude to the a posteriori uncertainty with the σΔXCH$_4$ ranging from an average of 9.6 ppb in summer to 14.5 ppb in winter compared to the a posteriori uncertainty that ranges from 6.6 ppb in summer to 10.8 ppb in winter. This suggests that regardless of the contribution to the uncertainty from the XCO$_2$ model, it would be difficult for the satellite data to inform the inversion any further than the in situ data already do. However, this is not the case for the North American Temperate region where the μΔXCH$_4$ (7.4–11.6 ppb) and σΔXCH$_4$ (8.4–10.0 ppb) are far larger than the total uncertainty (6.0–6.9 ppb) for much of the year. Both Southern Ocean regions exhibit more complicated behaviour with far less of an apparent seasonality in the μΔXCH$_4$. Instead, for most years μΔXCH$_4$ is much higher than the uncertainties (which themselves do not exhibit much seasonality in these regions). However, the year 2010 seems to be an anomalous year where the μΔXCH$_4$ data are much more in agreement and in this year the difference is of comparable magnitude to the uncertainties with values between 4 and 8 ppb. The σΔXCH$_4$ does exhibit more seasonality than the μΔXCH$_4$ and is again considerably higher than the estimated uncertainties (7–20 ppb vs. 5–6 ppb). In combination, this suggests that the GOSAT observations over Southern America should add considerable information to the inversion.

For Northern Africa, both the a posteriori error and the uncertainty related to the XCO$_2$ model are small due to the high SNR over the Sahara and the low CO$_2$ variability respectively (with seasonal average values ranging from 3.3 to 3.6 ppb for the a posteriori error and from 2.8 to 4.6 ppb for the model XCO$_2$ error). In contrast, the μΔXCH$_4$ (7.2–12.3 ppb) and σΔXCH$_4$ (4.9–8.4 ppb) values over this region are relatively large with a high degree of temporal variability, suggesting that the satellite data should add considerable value in constraining the inversion over this region. One complication is that GOSAT operates in a “medium gain” mode over the desert and hence may exhibit different instrumental biases over such regions but, due to the proxy method, any such differences in instrumental biases that relate to light-path modification should be minimised. Southern Africa shows similar behaviour with the total uncertainty being low (seasonal averages of 5.1–7.3 ppb) compared to the much larger μΔXCH$_4$ (12.6–19.8 ppb) and σΔXCH$_4$ (5.7–10.7 ppb) values, again indicating that considerable value is present in the satellite data.

The Eurasian Boreal region behaves similarly to the North American Boreal region. The μΔXCH$_4$ and σΔXCH$_4$ is of similar phase and magnitude to the retrieval a posteriori error, suggesting little information will be added to any inversion over this region beyond what is available from the in situ measurements. In contrast, the μΔXCH$_4$ values over the Eurasian Temperate region show a large variability with the differences in winter months much larger than the total uncertainty (9.9 ppb vs. 5.8 ppb), while in summer months the magnitudes become much more similar (5.5 ppb vs. 7.3 ppb). Interestingly, the σΔXCH$_4$ values appear to be of similar magnitude (5–20 ppb) but directly out of phase with the μΔXCH$_4$ values. Even during summer months when the a posteriori (4.3 ppb) and model XCO$_2$ (5.8 ppb) uncertainties are comparable to the μΔXCH$_4$ (5.5 ppb), the high variability in the ΔXCH$_4$ values, as indicated by σΔXCH$_4$ values of up to 20 ppb (and a summertime mean value of 15.0 ppb), suggests that the observations are capable of providing useful information to the inversion.
The Tropical Asian region, which encompasses parts of India, China, and Indonesia, typically has low values for both the a posteriori (5.6–6.9 ppb) and XCO$_2$ model (4.4–6.0 ppb) uncertainties, with neither exhibiting much seasonal variability. The $\mu_{\Delta XCH_4}$ and $\sigma_{\Delta XCH_4}$ values however are much more variable (8.9–11.7 and 9.0–16.8 ppb) and generally much higher than the uncertainties, suggesting that useful information from the satellite data is present.

The European Transcom region has uncertainties in the satellite data (seasonal averages of 7.6–10.0 ppb) that are of comparable magnitude to the $\mu_{\Delta XCH_4}$ values (8.1–10.7 ppb), especially when considering the combination of the a posteriori and model XCO$_2$ uncertainties. However, the standard deviation of the $\mu_{\Delta XCH_4}$ values is highly variable (8.7–13.2 ppb) which suggests that there is scope for the observational data to aid in constraining the European XCH$_4$ fluxes.

Finally, the Australian Transcom region shows very small uncertainties in the satellite data. The uncertainty associated with the model XCO$_2$ is comparable to the a posteriori error during the Australian spring months but even in those circumstances, the $\mu_{\Delta XCH_4}$ values are far larger (11.4 ppb vs. 4.7 ppb), demonstrating that the satellite data are capable of providing some information to the inversion over Australia, although this may be limited in its ability to provide specific information on Australian sources as the $\sigma_{\Delta XCH_4}$ values over this region are similar to the estimated uncertainties with seasonal averages of 4.5–5.2 ppb compared to the total uncertainty values of 4.1–5.0 ppb.

6 Summary and conclusions

We present details of the update to the University of Leicester GOSAT Proxy XCH$_4$ v5.0 data set with 5 years of GOSAT data now processed. The data are validated against the latest ground-based TCCON data and found to agree well with on average a small bias of 4.8 ppb ($\sim$0.27%), a single-sounding precision of 13.4 ppb ($\sim$0.74%), and a relative accuracy of 4.2 ppb. For the first time the XCH$_4$ / XCO$_2$ ratio component of the proxy retrieval is validated and also found to agree well with TCCON with a bias of 0.014 ppb ppm$^{-1}$ ($\sim$0.3 %) and a single-sounding precision of 0.033 ppb ppm$^{-1}$ ($\sim$0.72 %).

A major unknown uncertainty in previous Proxy XCH$_4$ products was the uncertainty associated with the model XCO$_2$. In this work we validate three separate state-of-the-art chemistry transport models against the TCCON data and find that although the models can differ greatly (>$4$ ppm) away from the TCCON stations, at the validation locations it is difficult to distinguish which model performs better from our comparisons. We therefore decide to use the median of the three models to act as the model XCO$_2$ in the calculation of the Proxy XCH$_4$ and use the maximum difference to the median as a measure of the uncertainty in the model XCO$_2$. This model uncertainty is found to vary greatly in time and space but is typically largest over regions associated with biomass burning such as central Africa and in particular over the Eurasian regions during summer months where large uptake in CO$_2$ leads to large differences between the models.
In order to assess the relative importance of these uncertainties, we compare this model XCO$_2$ uncertainty to the a posteriori retrieval error over the different Transcom regions and find typically that where there is seasonality in the uncertainties, it is typically directly out of phase between the two, resulting in the model XCO$_2$ uncertainty becoming significant during summer months where the a posteriori error is at its lowest. This relates to the fact that more sunlight leads to a reduction in the a posteriori uncertainty (by virtue of providing a greater signal in the SWIR) and at the same time is associated with an increase in photosynthesis and, hence, more potential for differences in the model XCO$_2$.

We assess the significance of these uncertainties on any flux inversion by comparing the mean and standard deviation of the GOSAT—MACC differences ($\mu_{\Delta XCH_4}$ and $\sigma_{\Delta XCH_4}$) to the estimated uncertainties. We find that for the majority of regions the mean and standard deviation of the $\Delta XCH_4$ values are much larger than the estimated uncertainties, even taking into account the uncertainty related to the model XCO$_2$. Our findings show that useful information will be provided to the inversions for the majority of regions, with the exceptions being the boreal regions (North American Boreal and Eurasian Boreal) where the uncertainty is of a similar magnitude to the $\mu_{\Delta XCH_4}$ and $\sigma_{\Delta XCH_4}$ values. It is important to note that the MACC data are already constrained by NOAA background sites.

One final consideration for users of the Proxy XCH$_4$ data who are performing atmospheric inversions is that, should they have their own XCO$_2$ model which they believe is consistent with their XCH$_4$ model, it may be beneficial to only take the GOSAT XCH$_4$ / XCO$_2$ ratio and apply their own model XCO$_2$ (with appropriate averaging kernels) in order to minimise transport model errors between the different models. Alternatively the XCH$_4$ / XCO$_2$ ratio can also be inverted directly as shown in Fraser et al. (2014) and Pandey et al. (2015).
Appendix A: Data sets

The GOSAT Proxy XCH$_4$ data used in this publication are freely available from http://www.leos.le.ac.uk/GHG/ghg_cci/CRDP/data_2/ESACCI/GHG/GOSAT/CH4_GOS_OCPR/5.1/ upon request of a password. An updated version of this data set is now available (version 6.0) covering 2009–2014. Additionally, these data now contain both the raw XCH$_4$ and XCO$_2$ values as well as the uncertainty associated with the model XCO$_2$.

The TCCON XCH$_4$ and XCO$_2$ data used in this publication are publicly available from http://tccon.ornl.gov. The following data have been used: Sodankylä (Kivi et al., 2014), Białystok (Deutscher et al., 2014), Karlsruhe (Hase et al., 2014), Orleans (Warneke et al., 2014), Garmisch (Sussmann and Rettinger, 2014), Park Falls (Wennberg et al., 2014a), Lamont (Wennberg et al., 2014b), Saga (Kawakami et al., 2014), Darwin (Griffith et al., 2014a), Wollongong (Griffith et al., 2014b), Lauder120 (Sherlock et al., 2014a), and Lauder125 (Sherlock et al., 2014b).
Table A1. Table showing the comparison statistics between each XCO₂ model (sampled as per the GOSAT measurements) within ±2σ of each TCCON site against the TCCON validation data. The difference (model–TCCON), the standard deviation of the difference, and the correlation coefficient are all provided as is the total number of measurements for each site, N, and the percentage “share” of the median for each model, %. For each of the three models, GEOS-Chem, MACC-II, and CarbonTracker, the best (bold) and worst (italic) value for each metric is highlighted. For the ensemble median data, all values which are better than the best individual model value are highlighted in bold-italic. The lower panel provides overall statistics across all sites. These include the relative accuracy (the standard deviation of the individual site biases), the overall precision (the standard deviation of the GOSAT–TCCON differences), and the overall share that each model contributes to the median ensemble.

| Region               | Season       | A posteriori (ppb) | Model (ppb) | Total (ppb) | \(\mu_\Delta XCH_4\) (ppb) | \(\sigma_{XCH_4}\) (ppb) | Region               | Season       | A posteriori (ppb) | Model (ppb) | Total (ppb) | \(\mu_\Delta XCH_4\) (ppb) | \(\sigma_{XCH_4}\) (ppb) |
|----------------------|--------------|-------------------|-------------|-------------|-----------------------------|-----------------------------|----------------------|--------------|-------------------|-------------|-------------|-----------------------------|-----------------------------|
| North America        | boreal       | spring            | 7.4         | 2.2         | 7.8                         | 6.3                         | 13.0                  | Eurasian      | spring            | 7.1         | 3.2         | 8.0                         | 4.5                         |
|                      |              | summer            | 6.6         | 4.9         | 8.3                         | 2.9                         | 9.6                   | boreal         | summer            | 6.3         | 7.0         | 9.5                         | 4.4                         |
|                      |              | autumn            | 10.0        | 2.8         | 10.5                        | 6.2                         | 11.4                  | autumn         | summer            | 4.3         | 5.8         | 7.3                         | 5.5                         |
|                      |              | winter            | 10.8        | 2.3         | 11.1                        | 11.5                        | 14.5                  | winter         | summer            | 4.4         | 4.1         | 6.2                         | 6.5                         |
|                      | temperate    | spring            | 5.1         | 3.0         | 6.0                         | 11.2                        | 9.2                   | Eurasian      | temperate         | 4.4         | 3.5         | 7.9                         | 11.7                        |
|                      |              | summer            | 4.6         | 4.7         | 6.4                         | 7.4                         | 8.6                   | temperate      | summer            | 4.3         | 5.8         | 7.3                         | 5.5                         |
|                      |              | autumn            | 5.3         | 3.1         | 6.3                         | 7.7                         | 8.4                   | autumn         | summer            | 4.4         | 4.1         | 6.2                         | 6.5                         |
|                      |              | winter            | 6.5         | 2.4         | 6.9                         | 11.6                        | 10.0                  | winter         | summer            | 5.2         | 2.6         | 5.8                         | 9.9                         |
| South America        | tropical     | spring            | 6.4         | 4.3         | 7.8                         | 8.6                         | 11.2                  | Tropical Asia  | spring            | 6.0         | 6.0         | 8.5                         | 8.9                         |
|                      |              | summer            | 5.3         | 4.3         | 6.9                         | 10.8                        | 8.6                   | summer         | summer            | 6.9         | 5.0         | 8.7                         | 10.9                        |
|                      |              | autumn            | 5.8         | 5.2         | 7.9                         | 10.7                        | 12.6                  | summer         | autumn            | 6.2         | 6.0         | 8.7                         | 11.7                        |
|                      |              | winter            | 6.5         | 4.1         | 7.8                         | 7.4                         | 15.5                  | winter         | summer            | 5.6         | 4.4         | 7.2                         | 10.9                        |
| South America        | temperate    | spring            | 4.7         | 3.7         | 6.1                         | 6.0                         | 10.7                  | Australia      | spring            | 3.9         | 2.5         | 4.7                         | 11.4                        |
|                      |              | summer            | 4.3         | 3.4         | 5.5                         | 9.1                         | 7.4                   | summer         | summer            | 3.7         | 1.8         | 4.1                         | 11.7                        |
|                      |              | autumn            | 4.2         | 3.7         | 5.7                         | 9.1                         | 9.7                   | autumn         | summer            | 3.7         | 2.1         | 4.3                         | 13.9                        |
|                      |              | winter            | 4.7         | 3.8         | 6.1                         | 7.2                         | 13.5                  | winter         | summer            | 4.2         | 2.5         | 4.0                         | 15.0                        |
| Northern Africa      |              | spring            | 3.6         | 3.6         | 5.2                         | 8.8                         | 7.3                   | Europe         | spring            | 6.7         | 3.5         | 7.6                         | 9.2                         |
|                      |              | summer            | 3.6         | 4.6         | 5.9                         | 7.2                         | 7.4                   | summer         | summer            | 5.9         | 5.3         | 8.0                         | 10.7                        |
|                      |              | autumn            | 3.4         | 3.5         | 4.9                         | 12.3                        | 8.4                   | autumn         | summer            | 7.5         | 3.0         | 8.2                         | 8.1                         |
|                      |              | winter            | 3.3         | 2.8         | 4.3                         | 8.0                         | 4.9                   | winter         | summer            | 9.4         | 3.1         | 10.0                        | 9.3                         |
| Southern Africa      |              | spring            | 4.7         | 4.6         | 6.7                         | 15.5                        | 9.9                   | Europe         | spring            | 6.7         | 3.5         | 7.6                         | 9.2                         |
|                      |              | summer            | 3.7         | 3.4         | 5.1                         | 12.6                        | 5.7                   | summer         | summer            | 5.9         | 5.3         | 8.0                         | 10.7                        |
|                      |              | autumn            | 4.8         | 3.7         | 6.1                         | 13.5                        | 9.8                   | autumn         | summer            | 7.5         | 3.0         | 8.2                         | 8.1                         |
|                      |              | winter            | 5.4         | 4.8         | 7.3                         | 19.8                        | 10.7                  | winter         | summer            | 9.4         | 3.1         | 10.0                        | 9.8                         |
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References

Alexe, M., Bergamaschi, P., Segers, A., Detmers, R., Butz, A., Hasekamp, O., Guerlet, S., Parker, R., Boesch, H., Frankenberg, C., Scheepmaker, R. A., Dlugokencky, E., Sweeney, C., Wofsy, S. C., and Kort, E. A.: Inverse modelling of CH$_4$ emissions for 2010–2011 using different satellite retrieval products from GOSAT and SCIAMACHY, Atmos. Chem. Phys., 15, 113–133, doi:10.5194/acp-15-113-2015, 2015.

Bergamaschi, P., Frankenberg, C., Meirink, J. F., Krol, M., Dentener, F., Wagner, T., Platt, U., Kaplan, J. O., Kort, E. A., Heinmann, M., Dlugokencky, E., J. D., and Goede, A.: Satellite cartography of atmospheric methane from SCIAMACHY on board ENVISAT: 2. Evaluation based on inverse model simulations, J. Geophys. Res.-Atmos., 112, D2304, doi:10.1029/2005JD006235, 2007.

Bergamaschi, P., Frankenberg, C., Meirink, J. F., Krol, M., Villani, M. G., Houweling, S., Frank, D., Edward, J. D., John, B. M., Luciana, V. G., Andres, E., and Ingeborg, L.: Inverse modeling of global and regional CH$_4$ emissions using SCIAMACHY satellite retrievals, J. Geophys. Res.-Atmos., 114, D22301, doi:10.1029/2009JD0012287, 2009.

Bergamaschi, P., Houweling, S., Segers, A., Krol, M., Frankenberg, C., Scheepmaker, R. A., Dlugokencky, E., Wofsy, S. C., Kort, E. A., Sweeney, C., Schuck, T., Breninkmeijer, C., Chen, H., Beck, V., and Gerbig, C.: Atmospheric CH$_4$ in the first decade of the 21st century: inverse modeling analysis using SCIAMACHY satellite retrievals and NOAA surface measurements, J. Geophys. Res.-Atmos., 118, 7350–7369, doi:10.1002/jgrd.50480, 2013.

Boesch, H., Baker, D., Connor, B., Crisp, D., and Miller, C.: Global characterization of CO$_2$ column retrievals from shortwave-infrared satellite observations of the Orbiting Carbon Observatory-2 Mission, Remote Sensing, 3, 270–304, doi:10.3390/rs3020270, 2011.

Bousquet, P., Ciais, P., Miller, J. B., Dlugokencky, E. J., Hauglustaine, D., A., Frignet, C., Van Der Werf, G. R., Peylin, P., Brunke, E., Carouge, C., Langerfeld, R. L., Lathiere, J., Papa, F., Ramonet, M., Schmidt, M., Steele, L. P., Tyler, S. C., and White, J.: Contribution of anthropogenic and natural sources to atmospheric methane variability, Nature, 443, 439–443, doi:10.1038/nature05132, 2006.

Buchwitz, M., Reuter, M., Schneising, O., Boesch, H., Guerlet, S., Dils, B., Aben, I., Armante, R., Bergamaschi, P., Blumenstock, T., Bovensmann, H., Brunner, D., Buchmann, B., Burrows, J., Butz, A., Chedin, A., Chevallier, F., Crevoisier, C., Deutscher, N., Frankenberg, C., Hase, F., Hasekamp, O., Heymann, J., Kaminski, T., Laeng, A., Lichtenberg, G., Maziere, M. D., Noël, S., Notholt, J., Orphal, J., Popp, C., Parker, R., Scholze, M., Sussmann, R., Stiller, G., Warneke, T., Zehner, C., Bril, A., Crisp, D., Griffith, D., Kuze, A., O’Dell, C., Oshchepkov, S., Sherlock, V., Suto, H., Wennberg, P., Wunch, D., Yokota, T., and Yoshida, Y.: The Greenhouse Gas Climate Change Initiative (GHG-CCI): comparison and quality assessment of near-surface-sensitive satellite-derived CO$_2$ and CH$_4$ global data sets, Remote Sens. Environ., 162, 344–362, doi:10.1016/j.rse.2013.04.024, 2013.

Butz, A., Hasekamp, O. P., Frankenberg, C., Vidot, J., and Aben, I.: CH$_4$ retrievals from space-based solar backscatter measurements: performance evaluation against simulated aerosol and cirrus loaded scenes, J. Geophys. Res.-Atmos., 115, D24302, doi:10.1029/2010JD014514, 2010.

Chevallier, F., Ciais, P., Conway, T., Aalto, T., Anderson, B., Bousquet, P., Brunke, E., Ciattaglia, L., Esaki, Y., Fröhlich, M., Gomez, A., Gomez-Pelaez, A., Haszpra, L., Krummel, P., Langerfelds, R., Leuenberger, M., MacFady, F., Matis, T., Murgui, J., Mukai, H., Nakazawa, T., Peylin, P., Ramon, M., Rivier, L., Sawa, Y., Schmidt, M., Steel, L., Vay, S., Vermeulen, A., Wofsy, S., and Worthy, D.: CO$_2$ surface fluxes at grid point scale estimated from a global 21 year reanalysis of atmospheric measurements, J. Geophys. Res.-Atmos., 115, D21307, doi:10.1029/2010JD013887, 2010.

Chipperfield, M. P.: Multiannual simulations with a three-dimensional chemical transport model, J. Geophys. Res.-Atmos., 104, 1781–1805, doi:10.1029/98JD02597, 1999.

Cogan, A., Boesch, H., Parker, R., Feng, L., Palmer, P., Blavier, J.-F., Deutscher, N. M., Macatangay, R., Notholt, J., Roehl, C., Warneke, T., and Wunch, D.: Atmospheric carbon dioxide retrieved from the Greenhouse gases Observing SATellite (GOSAT): comparison with ground-based TCCON observations and GEOS-Chem model calculations, J. Geophys. Res.-Atmos., 117, D21301, doi:10.1029/2012JD018087, 2012.

Connor, B. J., Boesch, H., Toon, G., Sen, B., Miller, C., and Crisp, D.: Orbiting Carbon Observatory: inverse method and prospective error analysis, J. Geophys. Res.-Atmos., 113, D05305, doi:10.1029/2006JD008336, 2008.
Cressot, C., Chevallier, F., Bousquet, P., Crevoisier, C., Dlugokencky, E. J., Fortems-Chiney, A., Frankenberger, C., Parker, R., Pison, I., Scheepmaker, R. A., Montzka, S. A., Krummel, P. B., Steele, L. P., and Langenfelds, R. L.: On the consistency between global and regional methane emissions inferred from SCIAMACHY, TANSO-FTS, IASI and surface measurements, Atmos. Chem. Phys., 14, 577–592, doi:10.5194/acp-14-577-2014, 2014.

Dee, D. P., Uppala, S. M., Simmons, A. J., Berrisford, P., Poli, P., Kobayashi, S., Andrae, U., Balsamo, G., Bauer, P., Bechtold, P., Beljaars, A. C. M., van de Berg, L., Bidlot, J., Bormann, N., Delsol, C., Dragani, R., Fuentes, M., Geer, A. J., Haimberger, L., Healy, S. B., Hersbach, H., Holm, E. V., Isaksen, L., Källberg, P., Köhler, M., Matricardi, M., Mcnally, A. P., Monge-Sanz, B. M., Morcrette, J.-J., Park, B.-K., Peubey, C., de Rosnay, P., Tavolato, C., Thépaut, J.-N., and Vitart, F.: The ERA-Interim reanalysis: configuration and performance of the data assimilation system, Q. J. Roy. Meteor. Soc., 137, 553–597, doi:10.1002/qj.828, 2011.

Deutscher, N., Notholt, J., Messerschmidt, J., Weinzierl, C., Warneke, T., Petri, C., Grupe, P., and Katrynski, K.: TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.bialystok01.R0/1149277, 2014.

Dils, B., Buchwitz, M., Reuter, M., Schneising, O., Boesch, H., Parker, R., Guerlet, S., Aben, I., Blumenstock, T., Burrows, J. P., Butz, A., Deutscher, N. M., Frankenberg, C., Hase, F., Hasekamp, O. P., Heymann, J., De Maziere, M., Notholt, J., Sussmann, R., Warneke, T., Griffith, D., Sherlock, V., and Wunch, D.: The Greenhouse Gas Climate Change Initiative (GHG-CCI): comparative validation of GHG-CCI SCIAMACHY/ENVISAT and TANSO-FTS/GOSAT CO2 and CH4 retrieval algorithm products with measurements from the TCCON, Atmos. Meas. Tech., 7, 1723–1744, doi:10.5194/amt-7-1723-2014, 2014.

Dlugokencky, E. J., Bruhwiler, L., White, J. W. C., Bousquet, P., Ciais, P., Saunois, M., Canadell, J. G., Kirschke, S., Bousquet, P., Ciais, P., Saunois, M., Canadell, J. G., Krummel, P. B., Langenfelds, R. L., O’Doherty, S., Prinn, R. G., Steele, L. P., van der Schoot, M., and Weiss, R. F.: Estimating regional methane surface fluxes: the relative importance of surface and GOSAT mole fraction measurements, Atmos. Chem. Phys., 13, 5697–5713, doi:10.5194/acp-13-5697-2013, 2013.

Fraser, A., Palmer, P. I., Feng, L., Böschi, H., Parker, R., Dlugokencky, E. J., Krummel, P. B., and Langenfelds, R. L.: Estimating regional fluxes of CO2 and CH4 using space-borne observations of XCH4: XCO2, Atmos. Chem. Phys., 14, 12883–12895, doi:10.5194/acp-14-12883-2014, 2014.

Griffith, D. W. T., Deutscher, N., Velazco, V. A., Wennberg, P. O., Yavin, Y., Aleks, G. K., Washenfelder, R., Toon, G. C., Blavier, J.-F., Murphy, C., Jones, N., Kettlewell, G., Connor, B., Macatangay, R., Roehl, C., Ryczek, M., Glocwaki, J., Culgan, T., and Bryant, G.: TCCON Data from Darwin, Australia, Release GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.darwin01.R0/1149290, 2014a.

Griffith, D. W. T., Velazco, V. A., Deutscher, N., Murphy, C., Jones, N., Wilson, S., Macatangay, R., Kettlewell, G., Buchholz, R. R., and Riggenbach, M.: TCCON Data from Wollongong, Australia, Release GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.wollongong01.R0/1149291, 2014b.

Gurney, K., Law, R., Denning, A., Rayner, P., Baker, D., Bousquet, P., Bruhwiler, L., Chen, Y.-H., Clas, P., Fan, S., Fung, I., Gloo, M., Heimann, M., Higuchi, K., John, J., Maki, T., Maksyutov, S., Masarie, K., Peylin, P., Prather, M., Pak, B., Randerson, J., Sarmineto, J., Taguchi, S., Takahashi, T., and Yuen, C.-W.: Towards robust regional estimates of CO2 sources and sinks using atmospheric transport models, Nature, 415, 626–630, doi:10.1038/415626a, 2002.

Hase, F., Blumenstock, T., Dohe, S., Groß, J., and Kiel, M.: TCCON Data from Karlsruhe, Germany, Release GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.karlsruhe01.R0/1149270, 2014.

Houweling, S., Krol, M., Bergamaschi, P., Frankenberg, C., Dlugokencky, E. J., Morino, I., Notholt, J., Sherlock, V., Wunch, D., Beck, V., Gerbig, C., Chen, H., Kort, E. A., Röckmann, T., and Aben, I.: A multi-year methane inversion using SCIAMACHY, accounting for systematic errors using TCCON measurements, Atmos. Chem. Phys., 14, 3991–4012, doi:10.5194/acp-14-3991-2014, 2014.

Kawakami, S., Ohyama, H., Arao, K., Okumura, H., Taura, C., Fukamachi, T., and Sakashita, M.: TCCON Data from Saga, Japan, Release GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.saga01.R0/1149283, 2014.

Kirschke, S., Bousquet, P., Ciais, P., Saunois, M., Canadell, J. G., Dlugokencky, E. J., Bergamaschi, P., Bergmann, D., Blake, D. R., Bruhwiler, L., Cameron-Smith, P., Castaldi, S., Chevallier, F., Feng, L., Fraser, A., Heimann, M., Hodson, E. L., Houweling, S., Josse, B., Fraser, P. J., Krummel, P. B., Lamarque, J.-
F., Langenfelds, R. L., Le Quere, C., Naik, V., O’Doherty, S., Palmer, P. I., Pison, I., Plummer, D., Poulter, B., Prinn, R. G., Rigby, M., Ringleval, B., Santini, M., Schmidt, M., Shindell, D. T., Simpson, I. J., Spahni, R., Steele, L. P., Strude, S. A., Sudo, K., Szopa, S., van der Werf, G. R., Voulgarakis, A., van Weele, M., Weiss, R. F., Williams, J. E., and Zeng, G.: Three decades of global methane sources and sinks, Nat. Geosci., 6, 813–823, 2013.

Kivi, R., Heikkinen, P., and Kyro., E.: TCCON Data from Sodankyla, Finland, Release GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.sodankyla01.R0/1149280, 2014.

Kuze, A., Taylor, T., Kataoka, F., Bruegge, C., Crisp, D., Harada, M., Helmlinger, M., Inoue, M., Kawakami, S., Kikuchi, N., Mitomi, Y., Murooka, J., Naitoh, M., O’Brien, D., O’Dell, C., Ohyama, H., Pollock, H., Schwandner, F., Shiotomi, K., Suto, H., Takeda, T., Tanaka, T., Urabe, T., Yokota, T., and Yoshida, Y.: Long-term varicous calibration of GOSAT short-wave sensors: techniques for error reduction and new estimates of radiometric degradation factors, IEEE T. Geosci. Remote, 52, 3991–4004, doi:10.1109/TGRS.2013.2278696, 2014.

Messerschmidt, J., Macatangay, R., Notholt, J., Petri, C., Warneke, T., and Weinzierl, C.: Side by side measurements of CO2 by ground-based Fourier transform spectrometer (FTS), Tellus B, 62, 749–758, doi:10.1111/j.1600-0889.2010.00491.x, 2010.

Monteil, G., Houweling, S., Butz, A., Guelet, S., Schepers, D., Hasekamp, O., Frankenberg, C., Scheepmaker, R., Aben, I., and Röckmann, T.: Comparison of CH4 inversions based on 15 months of GOSAT and SCIAMACHI observations, J. Geophys. Res.-Atmos., 118, 11807–11823, doi:10.1002/2013JD020176, 2013.

Myhre, G., Shindell, D., Bréon, F.-M., Collins, W., Fuglestvedt, J., Huang, J., Koch, D., Lamarque, J.-F., Lee, D., Mendoza, B., Nakajima, T., Robock, A., Stephens, G., Takemura, T., and Zhang, H.: Anthropogenic and natural radiative forcing, chap. 8, in: Climate Change 2013: the Physical Science Basis, Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change, edited by: Stocker, T., Qin, D., Plattner, G.-K., Tignor, M., Allen, S., Boschung, J., Nauels, A., Xia, Y., Bex, V., and Midgley, P., Cambridge University Press, 659–740, doi:10.1017/CBO9781107415324.018, 2013.

Nisbet, E., Dlugokencky, E., and Bousquet, P.: Methane on the rise – again, Science, 343, 493–495, doi:10.1126/science.1247824, 2014.

O’Dell, C. W., Connor, B., Bösch, H., O’Brien, D., Frankenberg, C., Castano, R., Christi, M., Eldering, D., Fisher, B., Gunson, M., McDuffie, J., Miller, C. E., Natraj, V., Oyafuso, F., Polonsky, I., Smyth, M., Taylor, T., Toon, G. C., Wennberg, P. O., and Wunch, D.: The ACOS CO2 retrieval algorithm – Part 1: Description and validation against synthetic observations, Atmos. Meas. Tech., 5, 99–121, doi:10.5194/amt-5-99-2012, 2012.

Pandey, S., Houweling, S., Krol, M., Aben, I., and Röckmann, T.: On the use of satellite-derived CH4 : CO2 columns in a joint inversion of CH4 and CO2 fluxes, Atmos. Chem. Phys., 15, 8615–8629, doi:10.5194/acp-15-8615-2015, 2015.
GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.orleans01.R0/1149276, 2014.

Wennberg, P. O., Roehl, C., Wunch, D., Toon, G. C., Blavier, J.-F., Washenfelder, R., Keppel-Aleks, G., Allen, N., and Ayers, J.: TCCON Data from Park Falls, Wisconsin, USA, Release GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.parkfalls01.R0/1149161, 2014.

Wennberg, P. O., Wunch, D., Roehl, C., Blavier, J.-F., Toon, G. C., Allen, N., Dowell, P., Teske, K., Martin, C., and Martin, J.: TCCON Data from Lamont, Oklahoma, USA, Release GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.lamont01.R0/1149159, 2014.

Wunch, D., Toon, G. C., Wennberg, P. O., Wofsy, S. C., Stephens, B. B., Fischer, M. L., Uchino, O., Abshire, J. B., Bernath, P., Biraud, S. C., Blavier, J.-F. L., Boone, C., Bowman, K. P., Browell, E. V., Campos, T., Connor, B. J., Daube, B. C., Deutscher, N. M., Diao, M., Elkins, J. W., Gerbig, C., Gottlieb, E., Griffith, D. W. T., Hurst, D. F., Jiménez, R., Keppel-Aleks, G., Kort, E. A., Macatangay, R., Machida, T., Matsueda, H., Moore, F., Morino, I., Park, S., Robinson, J., Roehl, C. M., Sawa, Y., Sherlock, V., Sweeney, C., Tanaka, T., and Zondlo, M. A.: Calibration of the Total Carbon Column Observing Network using aircraft profile data, Atmos. Meas. Tech., 3, 1351–1362, doi:10.5194/amt-3-1351-2010, 2010.

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

Wennberg, P. O., Roehl, C., Wunch, D., Toon, G. C., Allen, N., Dowell, P., Teske, K., Martin, C., and Martin, J.: TCCON Data from Park Falls, Wisconsin, USA, Release GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.parkfalls01.R0/1149161, 2014.

Wennberg, P. O., Wunch, D., Roehl, C., Blavier, J.-F., Toon, G. C., Allen, N., Dowell, P., Teske, K., Martin, C., and Martin, J.: TCCON Data from Lamont, Oklahoma, USA, Release GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.lamont01.R0/1149159, 2014.

Wunch, D., Toon, G. C., Wennberg, P. O., Wofsy, S. C., Stephens, B. B., Fischer, M. L., Uchino, O., Abshire, J. B., Bernath, P., Biraud, S. C., Blavier, J.-F. L., Boone, C., Bowman, K. P., Browell, E. V., Campos, T., Connor, B. J., Daube, B. C., Deutscher, N. M., Diao, M., Elkins, J. W., Gerbig, C., Gottlieb, E., Griffith, D. W. T., Hurst, D. F., Jiménez, R., Keppel-Aleks, G., Kort, E. A., Macatangay, R., Machida, T., Matsueda, H., Moore, F., Morino, I., Park, S., Robinson, J., Roehl, C. M., Sawa, Y., Sherlock, V., Sweeney, C., Tanaka, T., and Zondlo, M. A.: Calibration of the Total Carbon Column Observing Network using aircraft profile data, Atmos. Meas. Tech., 3, 1351–1362, doi:10.5194/amt-3-1351-2010, 2010.

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

Wennberg, P. O., Roehl, C., Wunch, D., Toon, G. C., Allen, N., Dowell, P., Teske, K., Martin, C., and Martin, J.: TCCON Data from Park Falls, Wisconsin, USA, Release GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.parkfalls01.R0/1149161, 2014.

Wennberg, P. O., Wunch, D., Roehl, C., Blavier, J.-F., Toon, G. C., Allen, N., Dowell, P., Teske, K., Martin, C., and Martin, J.: TCCON Data from Lamont, Oklahoma, USA, Release GGG2014R0. TCCON Data Archive, hosted by the Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA, doi:10.14291/tccon.ggg2014.lamont01.R0/1149159, 2014.

Wunch, D., Toon, G. C., Wennberg, P. O., Wofsy, S. C., Stephens, B. B., Fischer, M. L., Uchino, O., Abshire, J. B., Bernath, P., Biraud, S. C., Blavier, J.-F. L., Boone, C., Bowman, K. P., Browell, E. V., Campos, T., Connor, B. J., Daube, B. C., Deutscher, N. M., Diao, M., Elkins, J. W., Gerbig, C., Gottlieb, E., Griffith, D. W. T., Hurst, D. F., Jiménez, R., Keppel-Aleks, G., Kort, E. A., Macatangay, R., Machida, T., Matsueda, H., Moore, F., Morino, I., Park, S., Robinson, J., Roehl, C. M., Sawa, Y., Sherlock, V., Sweeney, C., Tanaka, T., and Zondlo, M. A.: Calibration of the Total Carbon Column Observing Network using aircraft profile data, Atmos. Meas. Tech., 3, 1351–1362, doi:10.5194/amt-3-1351-2010, 2010.