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Consistent evaluation of GOSAT, SCIAMACHY, CarbonTracker, and MACC through comparisons to TCCON

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Abstract

Consistent validation of satellite CO₂ estimates is a prerequisite for using multiple satellite CO₂ measurements for joint flux inversion, and for establishing an accurate long-term atmospheric CO₂ data record. We focus on validating model and satellite observation attributes that impact flux estimates and CO₂ assimilation, including accurate error estimates, correlated and random errors, overall biases, biases by season and latitude, the impact of coincidence criteria, validation of seasonal cycle phase and amplitude, yearly growth, and daily variability. We evaluate dry air mole fraction (X_{CO2}) for GOSAT (ACOS b3.5) and SCIAMACHY (BESD v2.00.08) as well as the Carbon-Tracker (CT2013b) simulated CO₂ mole fraction fields and the MACC CO₂ inversion system (v13.1) and compare these to TCCON observations (GGG2014). We find standard deviations of 0.9 ppm, 0.9, 1.7, and 2.1 ppm versus TCCON for CT2013b, MACC, GOSAT, and SCIAMACHY, respectively, with the single target errors 1.9 and 0.9 times the predicted errors for GOSAT and SCIAMACHY, respectively. When satellite data are

- ¹⁵ averaged and interpreted according to $\operatorname{error}^2 = a^2 + b^2/n$ (where *n* are the number of observations averaged, *a* are the systematic (correlated) errors, and *b* are the random (uncorrelated) errors), we find that the correlated error term *a* = 0.6 ppm and the uncorrelated error term *b* = 1.7 ppm for GOSAT and *a* = 1.0 ppm, *b* = 1.4 ppm for SCIA-MACHY regional averages. Biases at individual stations have year-to-year variability of
- ~ 0.3 ppm, with biases larger than the TCCON predicted bias uncertainty of 0.4 ppm at many stations. Using fitting software, we find that GOSAT underpredicts the seasonal cycle amplitude in the Northern Hemisphere (NH) between 46–53° N. In the Southern Hemisphere (SH), CT2013b underestimates the seasonal cycle amplitude. Biases are calculated for 3-month intervals and indicate the months that contribute to the observed
- amplitude differences. The seasonal cycle phase indicates whether a dataset or model lags another dataset in time. We calculate this at a subset of stations where there is adequate satellite data, and find that the GOSAT retrieved phase improves substantially over the prior and the SCIAMACHY retrieved phase improves substantially for





2 of 7 sites. The models reproduce the measured seasonal cycle phase well except for at Lauder125 (CT2013b), Darwin (MACC), and Izana (+ 10 days, CT2013b), as for Bremen and Four Corners, which are highly influenced by local effects. We compare the variability within one day between TCCON and models in JJA; there is correlation

⁵ between 0.2 and 0.8 in the NH, with models showing 10–100 % the variability of TC-CON at different stations (except Bremen and Four Corners which have no variability compared to TCCON) and CT2013b showing more variability than MACC. This paper highlights findings that provide inputs to estimate flux errors in model assimilations, and places where models and satellites need further investigation, e.g. the SH for models
 and 45–67° N for GOSAT.

1 Introduction

Carbon-climate feedbacks are a major uncertainty in predicting the climate response to anthropogenic forcing (Friedlingstein et al., 2006). Currently, about 9 Gigatons (Gt) of carbon are emitted per year from human activity (e.g. fossil fuel burning, deforestation), of which about 5 Gt stays in the atmosphere, causing an annual CO₂ increase of approximately 2 ppm yr⁻¹. The yearly increase is quite variable, estimated at 1.99 ± 0.43 ppm yr⁻¹ (http://www.esrl.noaa.gov/gmd/ccgg/trends/global.html), however always positive (Houghton et al., 2007). The remaining 4Gt of carbon is taken up by the ocean and the terrestrial biosphere, however there are uncertainties in the location and mechanism of these sinks, e.g. the distribution of land sinks between the Northern Hemisphere and the tropics (e.g. Stephens et al., 2007), and the localization of sources and sinks on regional scales (Canadell et al., 2011; Baker et al., 2006). The

- uncertainties in top-down source and sink estimates are a consequence of uncertainties in model transport and dynamics (e.g. Prather et al., 2008; Stephens et al., 2007) and sparseness of available surface-based CO₂ observations (Hungershoefer et al.,
- 2010; Chevallier et al., 2010). Satellites offer a much denser and spatially contiguous





dataset for top-down estimates, but are much more susceptible to biases as compared to ground-based measurements (e.g. see summary in Sect. 3.3.2 of Ciais et al., 2014).

This paper tests different characteristics of model and satellite CO₂ (e.g. seasonal cycle amplitude and phase, regional and seasonal biases, effects of averaging, and diurnal variations) through a series of specialized comparisons to the Total Carbon Column Observing Network (TCCON). The findings from this work can be propagated into assimilation systems to determine the influence of various findings on top-down flux estimates (e.g. see Miller et al., 2007; Deng et al., 2013; Chevallier and O'Dell, 2013; Chevallier et al., 2014). For example, this paper characterizes biases by lati-tude and season; these biases can be assimilated to determine their effects on flux estimates (e.g. Kulawik et al., 2013). These findings also apply to bottom-up flux estimates, for example, updates should be made in inventories or transport to correct the model fields at the TCCON stations showing seasonal cycle phase differences.

2 Data and models used

¹⁵ The characteristics of the sets of carbon dioxide that will be compared to TCCON are summarized in Table 1. The following sections contain detailed descriptions of the dataset versions and characteristics.

2.1 GOSAT CO₂

The Greenhouse gases Observing SATellite (GOSAT) takes measurements of reflected sunlight in three short-wave bands with a footprint of approximately 10.5 km at nadir (Yokota et al., 2009; Crisp et al, 2012). The first useable science measurements were made in April 2009, but due to changing observational modes in the early months, we use data beginning in July 2009. In this work, we use column averaged dry air mole fraction (X_{CO2}) retrievals produced by NASA's Atmospheric CO2 Observations
 ²⁵ from Space (ACOS) project, version 3.5 (see O'Dell et al., 2012, for retrieval details).





For each sounding, the retrieval produces an estimate of X_{CO_2} , the vertical sensitivity of the measurement (i.e., the averaging kernel), and the posterior uncertainty in X_{CO_2} . It also produces a number of other retrieval variables, such as surface pressure and aerosols, which are used in both filtering and bias-correction. Post-retrieval

- ⁵ filter is employed based on a number of variables associated with the retrieval. In addition to filtering, a revised bias-correction scheme has been developed for the v3.5 retrievals. This scheme is similar to the approach described in Wunch et al. (2011), which characterized the errors in earlier versions of the ACOS retrieval using a simple spatial uniformity assumption of X_{CO₂} in the Southern Hemisphere (sometimes re-
- ferred to as the "Southern Hemisphere Approximation") to assess errors and biases in the retrievals. V3.5 has corrections of GOSAT High (H) and Medium (M) gain data over land, as well as glint-mode data over the ocean, by using not only the "Southern Hemisphere Approximation", but also TCCON observations, and comparisons to an ensemble mean of multiple transport model output. Details of the post-retrieval filter and the bias-correction scheme can be found in the ACOS v3.5 user's guide which will
- soon be at https://co2.jpl.nasa.gov/.

2.2 SCIAMACHY CO₂

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The following description of the SCanning Imaging Absorption SpectroMeter for Atmospheric ChartographY (SCIAMACHY) CO_2 retrieval algorithm summarizes important aspects of Reuter et al. (2010, 2011) and is adopted in parts from the algorithm theoretical basis document (Reuter et al., 2012b).

The Bremen Optimal Estimation DOAS (BESD) algorithm is designed to analyze SCIAMACHY sun normalized radiance measurements to retrieve the column-average dry-air mole fraction of atmospheric carbon dioxide (X_{CO_2}). BESD is a so-called full physics algorithm, which uses measurements in the O₂-A absorption band to retrieve

scattering information of clouds and aerosols. This information is transferred to the CO_2 absorption band at 1580nm by simultaneously fitting the spectra measured in both spectral regions. Similar to the ACOS three-band retrieval for GOSAT, the explicit





consideration of scattering by this approach reduces potential systematic biases due to clouds or aerosols.

The retrieved 26-elements state vector consists of a second order polynomial of the surface spectral albedo in both fit windows, two instrument parameters (spectral shift
and slit functions full width at half maximum (FWHM) in both fit windows, described in Reuter et al., 2010), a temperature profile shift, a scaling of the H₂O profile and a default aerosol profile, cloud water/ice path, cloud top height, surface pressure and a ten layer CO₂ mixing ratio profile. Even though the number of state vector elements (26) is smaller than the number of measurement vector elements (134), the inversion problem is generally under-determined, especially for the CO₂ profile. For this reason BESD uses a priori knowledge as a side-constraint. However, for most of the state vector elements the a priori knowledge gives only a weak constraint and is therefore not dominating the retrieval results. The degree of freedom for X_{CO2} typically lies within an interval between 0.9 and 1.1.

- ¹⁵ A post-processor adjusts the retrieved X_{CO2} to a priori CO₂ profiles generated with the simple empirical CO₂ model (SECM) described by Reuter et al. (2012a). Additionally the post-processor performs quality filtering and bias correction. The bias correction is based on, e.g., convergence, fit residuals, error reduction, etc. The bias correction follows the idea of Wunch et al. (2011) using TCCON as reference to derive ²⁰ an empirical bias model depending on solar zenith angle, retrieved albedo, etc. The theoretical predicted errors have been scaled by 0.22 to agree with the errors versus
- theoretical predicted errors have been scaled by 0.22 to agree with the errors versus TCCON (Reuter et al., 2011). More details can be found in BESD's algorithm theoretical basis document (Reuter et al., 2012b).

2.3 The TCCON

²⁵ The Total Carbon Column Observing Network (TCCON) consists of ground-based Fourier transform spectrometers (FTS) that measure high spectral (0.02 cm^{-1}) and temporal (~90 s) resolution spectra of the direct sun in the near infrared (Wunch et al., 2011a). Column abundances of CO₂, O₂ and other atmospheric gases are determined





from their absorption signatures in the solar spectra using the GGG software package, which employs a nonlinear least squares spectral fitting algorithm to scale an a priori volume mixing ratio profile. Absorption of CO_2 is measured in the weak CO_2 band centered on 6220 and 6339 cm⁻¹, and of O_2 in the band centered on 7885 cm⁻¹.

The total column dry-air mole fractions of CO₂ (X_{CO₂}) are computed by ratioing the column abundances of CO₂ and O₂. The resulting dry-air mole fractions have been calibrated against profiles of CO₂ measured by WMO-scale instrumentation aboard aircraft (Wunch et al., 2010; Messerschmidt et al., 2011). The precision and accuracy of the TCCON X_{CO₂} product is ~ 0.8 ppm (2-sigma) after calibration (Wunch et al., 2010). The TCCON data used in this paper are from the GGG2012 release, available from http://tccon.ipac.caltech.edu/.

We use 18 TCCON stations, distributed globally (see Fig. 1), and these data have been used extensively for satellite validation (e.g., Butz et al., 2011; Morino et al., 2011; Wunch et al., 2011b; Reuter et al., 2011; Schneising et al., 2012; Oshchepkov

- et al., 2012), in flux inversions (Chevallier et al., 2011), and in model comparisons (Basu et al., 2011; Saito et al., 2012). We use the GGG2014 data when available, and the GGG2012 data from sites Four Corners, Tsukuba, and Bremen. The GGG2012 sites have corrections based on the instructions from the TCCON partners, listed on the TCCON website (https://tccon-wiki.caltech.edu/Network_Policy/Data_Use_Policy/
- Data_Description_GGG2012#Laser_Sampling_Errors). We also apply a 0.9972 factor to Four Corners, as indicated here: https://tccon-wiki.caltech.edu/Network_Policy/Data_Use_Policy/Data_Description_GGG2012. Two instruments have been operated at the Lauder site. We identify them using 120HR (for the 20 June 2004 through 28 February 2011 period) and 125HR (for 2 February 2010- through to the present) when results are instrument specific.

2.4 CarbonTracker

CarbonTracker (CT) is an annually-updated analysis of atmospheric carbon dioxide distributions and the surface fluxes that create them (Peters et al., 2007). Carbon-





Tracker uses the Transport Model 5 (TM5) offline atmospheric tracer transport model (Krol et al., 2005) driven by meteorology from the European Centre for Medium-Range Weather Forecasts (ECMWF) operational forecast model and from the ERA-interim reanalysis (Dee et al., 2011) to propagate surface emissions. TM5 runs at a global 3° × 2° resolution and at a 1° × 1° resolution over North American. CarbonTracker separately propagates signals from fossil fuel emissions, air-sea CO₂ exchange, and terrestrial fluxes from wildfire emissions and non-fire net ecosystem exchange. Similar to other existing CO₂ inverse models, oceanic and terrestrial biosphere surface fluxes are optimized to agree with atmospheric CO₂ observations, while fossil fuel and wildfire emissions.

- sions are specified. First-guess fluxes from terrestrial biosphere models and surface ocean carbon analyses are modified by applying weekly multiplicative scaling factors estimated for 126 land and 30 ocean regions using an ensemble Kalman filter optimization method. The CT2013b release of CarbonTracker assimilates in situ observations between 2000 and 2012 from 103 datasets around the world, including time series
- ¹⁵ from NOAA observatories, tall towers, and flasks sampled by the NOAA Cooperative Air Sampling Network, and flask and continuous measurements from partners including Environment Canada, the Australian Commonwealth Scientific and Industrial Research Organization (CSIRO), the National Center for Atmospheric Research (NCAR), the Lawrence Berkeley National Laboratory, and the Brazilian Instituto de Pesquisas-Energétiane e Nuclearee

20 Energéticas e Nucleares.

In order to explicitly quantify the impact of transport uncertainty and prior flux model bias on inverse flux estimates from CarbonTracker, the CT2013b release is composed of a suite of inversions, each using a different combination of prior flux models and parent meteorological model. Sixteen independent inversions were conducted, using

two terrestrial biosphere flux priors, two air-sea CO₂ exchange flux priors, two estimates of imposed fossil fuel emissions, and two transport estimates in a factorial design. CT2013b results are presented as the performance-weighted mean of the inversion suite, with uncertainties including a component of across-model differences.



All CarbonTracker results and complete documentation can be accessed online at http://carbontracker.noaa.gov.

For model-data comparisons at selected sites, CT2013b is sampled at 90-minute intervals on the model's native vertical grid of 34 levels. Quantities are laterally interpolated from grid points to the location of the site using the sub-grid tracer distribution model of the Russel and Lerner (1981) advection scheme. This "column" output includes CO₂ tracers and meteorological conditions, and is available online at ftp://aftp.cmdl.noaa.gov/products/carbontracker/co2/CT2013/column/.

2.5 MACC

- Monitoring Atmospheric Composition and Climate (MACC. http://www. 10 gmes-atmosphere.eu/) is the European Union-funded project responsible for the development of the pre-operational Copernicus atmosphere monitoring service. MACC monitors the global distributions of greenhouse gases, aerosols, and reactive gases, and estimates some of their sources and sinks. Since 2010, it has been delivering every year an analysis of the carbon dioxide in the atmosphere and of its surface fluxes, based on the assimilation of air sample mole fraction measurements (Chevallier et al., 2010). It relies on a variational inversion formulation, developed by LSCE, that estimates 8-day grid-point daytime/nighttime CO₂ fluxes and the grid point total columns of CO₂ at the initial time step of the inversion window. The Bayesian error statistics of the estimate are computed by a robust randomization approach. The MACC inversion scheme relies on the global tracer transport model LMDZ (Hourdin et al., 2006), driven by the wind analyses from the ECMWF. For release v13.1 of the MACC inversion, used here, LMDZ was run at a horizontal resolution 3.75° longitude × 1.9° latitude with 39 vertical layers. The other elements of the inversion
- ²⁵ configuration follow Chevallier et al. (2011), with climatological (i.e. not interannually-varying) terrestrial and ocean prior fluxes and interannually-varying fossil-fuel and biomass-burning emissions. The variational formulation of the inversion allowed the 1979–2013 period to be processed in a single assimilation window, therefore ensuring





the physical and statistical consistency of the inversion over the full 35-year period. Mole fraction records from 131 measurement sites have been used from the NOAA Earth System Research Laboratory archive, the World Data Centre for Greenhouse Gases (WDCGG) archive and the Réseau Atmosphérique de Mesure des Composés
à Effet de Serre (RAMCES) database (see the list in the Supplement of Peylin et al., 2013).

3 Direct comparisons to TCCON

We show comparisons between satellite X_{CO_2} , model simulated mole fraction fields and TCCON X_{CO_2} at 17 different TCCON sites, shown in Fig. 1. These sites span the Northern and Southern Hemispheres and cover a wide range of latitudes and longi-10 tudes, though not covering South America, and Africa, or Asia excepting Japan. Newer sites are not used as the coverage of SCIAMACHY dataset ends in mid-2012 and our version of CarbonTracker (CT2013b) ends at the end of 2012. We show representative time series for CT2013b, MACC, GOSAT, SCIAMACHY for a Northern Hemisphere site (Lamont, OK, US at 37° N) and two Southern Hemisphere sites (Lauder, 15 NZ at 45° S or Wollongong, New South Wales, Australia at 35° S) in Fig. 2. These plots show matches using the geometric coincidence criteria described in Table 2 below (for satellites) and give an idea of the number of coincidences for each dataset using these criterion. These sites were chosen as they have the most coincidences in the Northern and Southern Hemisphere, respectively, for satellites. All sets compare 20 well; the 30-day moving averages show differences most easily; such as a repeating blip in CT2013b comparisons at the summer drawdown at Lamont and a seasonal

blip in CT2013b comparisons at the summer drawdown at Lamont and a seasonal mismatches in CT2013b comparisons to Lauder, which will be discussed later in the paper.





3.1 Coincidence criteria and other matching details

The SCIAMACHY and GOSAT comparisons in this paper are based on two different definitions of coincidence criteria between TCCON and satellite data. Satellite measurements, which satisfy the so-called geometric criteria, are within ± 1 h, $\pm 5^{\circ}$ latitude and longitude of the mean time of a 90-min TCCON average. The dynamical criteria (Wunch et al., 2011; Keppel-Aleks et al., 2011, 2012) are designed to exploit information about the dynamical origin of an air parcel through a constraint on the free-tropospheric temperature. This allows us to relax the geometric constraints and find more coincident satellite soundings per TCCON measurement. Briefly, a match is found when the measurements are within 5 days and the following is satisfied:

$$\left(\left(\frac{\Delta \text{Latitude}}{10}\right)^2 + \left(\frac{\Delta \text{Longitude}}{30}\right)^2 + \left(\frac{\Delta \text{Temperature}}{2}\right)^2\right) < 1, \tag{1}$$

where Δ Temperature is the co-located NCEP temperature difference at 700 hPa (Kalnay et al., 1996). Table 2 summarizes the coincidence criteria and data versions that are used. Other matching schemes not included in this paper include a method implemented by S. Basu described in Guerlet et al. (2013), which utilizes model CO₂ fields to determine coincidences and Nguyen et al. (2013) which uses a weighted average of distance, time, and mid-Tropospheric temperature. Dynamic and geometric coincidence criteria are compared in Sect. 3.3 and geometric coincidence criteria are used to spot-check dynamic coincidence criteria results.

- The choices used in this paper regarding model/TCCON matchups are: linearly interpolating to the TCCON latitude, longitude, and time for MACC, interpolating to the TCCON time from the special CarbonTracker output that has been interpolated to the TCCON locations, and using the TCCON surface pressure for calculating X_{CO_2} . In the cases where the TCCON surface pressure is greater than the model surface pressure,
- the model surface CO_2 value is replicated to the missing pressure values.





3.2 Bias and standard deviation for individual matches

Figure 3 shows a summary of the comparisons for geometric criteria where satellite matches are not averaged. Averaging and the effects of coincidence criteria and satellite averaging are addressed in Sect. 3.4. The black box shows 5 European stations
which are very close, geographically, yet have different biases. The gray bars labeled "TCCON Bias Uncertainty" in Fig. 3 are estimated to be 0.4, the overall calibration uncertainty in TCCON (Wunch et al., 2010, 2011). When the measured biases are larger than the gray box, they are considered significantly different than TCCON. For GOSAT, biases larger than the TCCON bias uncertainty occur at stations north of 67° N (European Stations Versa), Garmisch, Four Corners, Tsukuba, and Lauder. Stations which have special circumstances regarding validation are: Garmisch which is in the midst of complicated terrain that is difficult to model local atmospheric transport and to measure from space; Four Corners (4C), which is located in the vicinity of two power plants with large CO₂ emissions (Lindenmaier et al., 2014). The meteorology is such that 4C reg-

- ¹⁵ ularly samples large localized plumes with column CO₂ increases of several ppm that last hours in the late morning. Therefore, the low bias in models and satellite data relative to the 4C TCCON is attributed to the smaller scale enhancements from the power plants measured in TCCON which are significantly diluted in the model and satellite results; Bremen is also affected by local urban sources, and satellites and models would
- ²⁰ be expected to be biased low; which is a finding, though it is similar to adjacent stations; and JPL is in a megacity with complex adjacent terrain. SCIAMACHY has the same outliers as GOSAT with an additional low bias at Karlsruhe. The models show similar biases to GOSAT and SCIAMACHY at stations north of 67° N (Eureka, Ny Alesund, Sodannkyla), Garmisch, Four Corners, but not at Tsukuba or Lauder. MACC
- additionally shows a low bias at JPL where the model scale does not allow resolution of this site. The standard deviation is shown in the right panel of Fig. 3. For unaveraged results, model standard deviations are lower than either satellite as satellite differences result from both systematic and random measurement error, the latter which does not





occur for models. The standard deviations show some variability from station to station which are investigated below. The effects of averaging and coincident criteria are investigated in Sect. 3.3.

- Figure 4 shows the biases and standard deviations grouped globally and over the
 northern and Southern Hemispheres. To estimate the overall bias and standard deviations for single observations, we take out the outliers as follows. For the models, we take out JPL, Four Corners, Bremen, and Garmisch, with the caveat that models are unable to resolve variations with complex orography (Garmisch) or strongly influenced by local sources (JPL, Four Corners, Bremen) due to resolution, and Tsukuba
 for the standard deviation, as the TCCON instrument at Tsukuba has higher standard deviation. For satellites, we remove the above plus Tsukuba and Lauder due to limited
- numbers of comparisons for SCIAMACHY. For the bias we take out stations poleward of 60° N, which have large positive biases for GOSAT and SCIAMACHY, which we note as an issue. There is an overall bias versus TCCON on the order of 0.7 ppm for
- ¹⁵ CT2013b, and 0.2–0.3 ppm for the other 3 sets. The overall bias is less of a concern than the bias variability in satellite data which indicates regional errors that will translate to regional errors in flux estimates. The bias variability is 0.4, 0.4, 0.5, and 0.3 ppm for CT2013b, MACC, SCIAMACHY, and GOSAT respectively. Note SCIAMACHY data are corrected to have an average zero bias with respect to TCCON GGG2012 which
- ²⁰ is 0.3 ppm higher than GGG2014 (https://tccon-wiki.caltech.edu/Network_Policy/ Data_Use_Policy/Data_Description#CORRECTIONS_AND_CALIBRATIONS). When stations north of 67° N and other large outliers and are excluded, the bias variability is on the order of the TCCON bias uncertainty of 0.4 ppm. The overall standard deviations are 0.9 ppm for CT2013b, 0.9 ppm for MACC, 2.1 ppm for SCIAMACHY, and 1.7 ppm
- for GOSAT. These values represent the overall performance of CT2013b, MACC, and single soundings from SCIAMACHY and GOSAT. The standard deviations are somewhat lower for the SH stations used, with values of 0.8, 0.8, 2.0, and 1.6 for CT2013b, MACC, SCIAMACHY, and GOSAT, respectively. Reuter et al. (2013) validated earlier retrieval versions of BESD-SCIAMACHY and ACOS-GOSAT with TCCON and found





2.1 ppm (BESD) and 2.3 ppm (ACOS) for the single sounding precision and 0.9 ppm for the station-to-station biases. Their findings for BESD are consistent with the findings of Dils et al. (2014). The station-to-station biases are lower in our analysis due to corrections in TCCON, improvements in satellite estimates, and removal of several stations from the estimates.

We test whether the biases seen in Figs. 3 and 4 are persistent from year to year. When at least two full-year averages exist for a station, the standard deviation of the yearly bias is calculated. The average over all stations of the yearly bias standard deviation is 0.3 ppm for all sets (CT2013b, MACC, SCIAMACHY, GOSAT). The year-to-year variability in the bias could be partly attributed to the distribution of data seasonally.

- year variability in the bias could be partly attributed to the distribution of data seasonally. Stations which have absolute biases more than 0.3 ppm different than the mean bias therefore have biases that are persistent from year to year. The stations which do not show biases are: GOSAT: Bialystok, Karlsruhe, Lamont, Izana. SCIAMACHY: Lamont. CT2013b: Ny Alesund, Orleans, Izana, Darwin, Wollongong, Lauder (both). MACC: Ny
 Alesund, Orleans, Park Falls, Lamont, Izana, Darwin, Wollongong, Lauder (both).
- Another important comparison is of the predicted and actual errors. The predicted error (also referred to as the a posteriori error) is reported for each satellite product and the actual error we take to be the standard deviation of the satellite observation versus TCCON. These two quantities should agree if the TCCON error is much smaller than
- the a posteriori error and the coincidence criteria does not degrade the agreement. The predicted and actual errors vary from site to site, e.g. from variations in albedo, aerosol composition, solar zenith angle, etc. We calculate the correlation between the standard deviation vs. TCCON and the predicted error for each site as follows: the standard deviation of the satellite vs. TCCON is calculated at each TCCON station.
- The correlation of the vectors of standard deviation and predicted errors by station are calculated. ACOS-GOSAT has a 0.6 correlation and BESD-SCIAMACHY has a 0.5 correlation. This indicates that the predicted error should be utilized, e.g. when assimilating ACOS-GOSAT, as the variability in the predicted error represents variability in the actual error, though not perfectly. A scale factor should also be applied to the



predicted errors. For ACOS-GOSAT the predicted error averaged over all TCCON sites is 0.9 ppm, as compared to the actual error of 1.7 ppm and can be corrected by applying a factor 1.9 to the reported GOSAT errors. For BESD-SCIAMACHY, the prediction error of 2.3 ppm multiplied by 0.9° with the 2.1 ppm actual error.

5 3.3 Errors as a function of coincidence criteria and averaging

We now directly compare performance of geometric and dynamic coincidence criteria and averaging in terms of error. Figure 5 shows SCIAMACHY and GOSAT standard deviations versus TCCON for geometric and dynamical coincidence criteria. The stations used were those that had entries for all comparisons, listed in the Fig. 5 caption. For n = 1 no averaging is done and the dynamic coincidence criteria performs similarly to

- the geometric criteria, though the dynamic error is ~ 0.2 ppm higher for SCIAMACHY. For n = 2, exactly two satellite observations were averaged for each coincidence. The error drops substantially, but not as $1/\sqrt{2}$, which would be expected if the error were uncorrelated. For n = 4, the error again drops but it is not half the n = 1 error, which is
- ¹⁵ shown by the dotted line. At n = 4, the dynamic coincidence criteria is the same as the geometric error, likely because dynamic coincidence involves averaging observations farther apart in location and time, which are less likely to have correlated errors. The last bar is the maximum n, which has results for all stations included. The dynamic criteria allows far more coincidences, resulting in significantly lower average errors. The
- 20 dynamic criteria is used for the remainder of the paper but with checks using the geometric criteria to ensure that artifacts are not added by the dynamic criteria. Note that all averaged satellite observations match to one particular TCCON observation.

3.4 Errors versus averaging: random and correlated error

To test the effects of spatial averaging, we calculate station by station standard deviations of satellite – TCCON matched pairs as a function of n, where n is the number of satellite observations that are averaged, which are chosen randomly from available





matches (so there should be no difference in the characteristics of chosen points for larger vs. smaller n). Figure 6 shows plots from Lamont for SCIAMACHY and GOSAT for standard deviation difference to TCCON versus n. Initially the error drops down rapidly with n, however the decrease slows with larger n. The curve fits well to the theoretically expected form:

$$\operatorname{error}^2 = a^2 + b^2/n,$$

where *a* represents correlated errors which do not decrease with averaging for similar cases (including smoothing errors, errors from interferents such as aerosols, TCCON error, and co-location error), *b* represents uncorrelated errors which decrease with averaging, and *n* represents the number of satellite observations that are averaged. The purple dashed line represents the standard deviation of CT2013b at the satellite time and location vs. CT2013b at the TCCON time and location. The purple dashed line represents spatio-temporal mismatch error and as expected, this value is much smaller for geometric than for dynamic coincidence criteria.

- ¹⁵ We calculate *a* and *b* by station in Table 3 with average values for northern hemispheric stations of $a = 1.5 \pm 0.3$ ppm, $b = 1.6 \pm 0.2$ ppm for SCIAMACHY geometric, $a = 1.1 \pm 0.2$ ppm, $b = 1.4 \pm 0.4$ ppm for SCIAMACHY dynamic, $a = 0.9 \pm 0.2$ ppm, $b = 1.7 \pm 0.3$ ppm for GOSAT dynamic. These values indicate the expected error when averaging GOSAT or SCIAMACHY observations matching to a single TCCON obser-
- vation. There is more correlated error, *a*, for SCIAMACHY geometric versus dynamic matches in 4/7 stations in the Northern Hemisphere, indicating that averaging is more effective when it is over a larger spatial/temporal area, probably due to variability in the source of the correlated errors. GOSAT only has two stations, Lamont and Park Falls, which have enough co-locations to directly compare dynamic and geometric coinci-
- ²⁵ dence criteria but these stations have smaller correlated error for geometric matches, which is true in all seasons. This could be due to the smaller GOSAT footprint allowing more variability from observation to observation. The co-locations error are ~ 0.3, 0.7, and 0.7 ppm, for SCIAMACHY geometric, SCIAMACHY dynamic, and GOSAT dy-



(2)



namic coincidences, respectively, based on model-model standard deviations between CT2013b at satellite versus TCCON locations/times. Correcting for the co-location error (CT-CT column in Table 3) and TCCON error (Appendix A) results in a = 1.4, 1.0, and 0.6 ppm for SCIAMACHY geometric, SCIAMACHY dynamic, GOSAT dynamic, re-

- ⁵ spectively. The correlated errors indicate a likely regional bias for the specified spatiotemporal scale, e.g. one would expect an error of 0.6 ppm for $5 \times 5^{\circ} \times 1$ h GOSAT averages. The larger *a* value for SCIAMACHY could be a result of the SCIAMACHY larger footprint size and closer footprints; which likely have more correlations in clouds, aerosols, and other sources of systematic errors versus the smaller, more separated,
- ¹⁰ GOSAT footprint which would likely have more variability in interferents from observation to observation.

The green dashed line in Fig. 6 shows the standard deviation of the satellite prior versus TCCON. Although using an optimal constraint will result in an error lower than the prior error in the absence of systematic errors, these satellite retrievals of CO_2 have been set up to value average results over single observations, so the error increases from the prior for a single observation, but average results have both less error and

3.5 Seasonal-dependent biases

minimal prior influence.

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It is important to determine whether there are seasonally-dependent biases, as these will impact flux distributions. We look at 3-months periods (DJF, MAM, JJA, SON), with the overall yearly bias at each site subtracted out to isolate the seasonal biases. To get enough comparisons, we use the dynamical criteria for satellite coincidences, as using the geometric criteria cuts down the comparisons with sufficient seasonal coverage to 3 stations (Park Falls, Lamont, and Wollongong).

Figure 7 shows the biases for stations that have at least 20 matches in each season, and Fig. 8 shows the results averaged by SH, $0-45^{\circ}$ N, $>45^{\circ}$ N. The error bars shown in Fig. 8 are the standard deviation of the results in each bin. Presumably when the bias is larger than the error bar, the bias is significant; we additionally tested the biases





for different years and compared the error bars to errors calculated using the bootstrap method (Rubin, 1981), the standard deviation of results within one bin, and differences in results when using dynamic vs. geometric coincidence criteria. Where results are available, we compared to geometric coincidence criteria. The persistent biases were that for 0–45° N SCIAMACHY is high in MAM, low in JJA, on the order of 1.2 ppm total spread; poleward of 45° N GOSAT and SCIAMACHY are low in DJF and high in JJA on the order of 0.8 ppm for SCIAMACHY and 0.4 ppm for GOSAT, and MACC is high in DJF and low in SON on the order of 0.3 ppm. Since the CO₂ peak occurs in MAM and the CO₂ minimum occurs in JJA, it would follow that the seasonal cycle amplitude bias should be about bias JJA - bias MAM. So these findings would indicate that 10 (1) SCIAMACHY should overestimates the seasonal cycle from $0-45^{\circ}$ N by ~ 1.2 ppm. Looking ahead to Sect. 4 and Table 4, SCIAMACHY overestimates the seasonal cycle amplitude from 0-45° N by 0.8 ppm. (2) GOSAT should underestimate the seasonal cycle > 45° N by 0.3 ppm. We find it overestimates by 0.9 ppm, and (3) MACC should overestimate the seasonal cycle north of 45° N by 0.3 ppm. We find it overestimates 15 by 0.1 ppm for 46–53° N and 0.3 for 67–79° N, however within the predicted errors. The seasonal biases are generally consistent with the seasonal cycle amplitude differences

versus TCCON and can be used to pinpoint which months cause the seasonal cycle amplitude differences versus TCCON.

In the SH, the seasonal biases are much small than in the NH. The seasonal cycle in the SH has its maximum in the October to January timeframe and minimum in the April timeframe. Looking at DFJ minus MAM biases should give the seasonal bias, which should be about + 0.5 for GOSAT and SCIAMACHY, -0.5 for CT2013b, and -0.2 for MACC. The signs and magnitudes are consistent with Table 4, given the error bars.

²⁵ 4 Comparisons of seasonal cycle amplitude, phase, and yearly increase

We compare to TCCON using the NOAA fitting software CCGCRV (Thoning et al., 1989) to calculate seasonal cycle amplitudes and yearly increases. At least 2 years are





needed to distinguish the seasonal cycle from the yearly increase. The errors are calculated using the bootstrap method (Rubin, 1981) and the standard deviation of results within one bin. Two datasets at a time are matched, using the dynamic criteria, with the satellite averaging 4 observations for SCIAMACHY and 2 for GOSAT, which reduces

- the fit errors. Since different datasets will have different data gaps and time ranges, the TCCON results will be somewhat different for each comparison. Plots are individually examined to ensure that there is adequate data (e.g. see Fig. 9). Stations that are removed are Tsukuba, Four Corners, and JPL2007, which do not have more than 2 years, Izana, Lauder, and Darwin for Sciamachy. Izana is removed because Izana is
- an ocean station and SCIAMACHY only retrieves over land. The ocean/land behavior is very different near Izana (see Fig. 10) and although the dynamic coincidence criteria does remarkably well with SCIAMACHY at Izana, it does not seem correct to include it, although the characteristics relative to TCCON are similar to Lamont for SCIAMACHY. The seasonal cycle amplitude is taken to be the maximum and minimum of the sam pled harmonic fit. This provides the best average seasonal amplitude over the time

4.1 Seasonal cycle amplitude

range.

The seasonal cycle amplitude is important for estimating source and sink estimates and global distributions. Table 4 shows the seasonal cycle amplitudes grouped by lat-

- itude. The errors represent the maximum of the predicted errors using the bootstrap method or the standard deviation of all results in that bin divided by the square root of the number of entries in that bin (*n*). All datasets show a similar pattern with respect to NH vs. SH, and with amplitudes increasing poleward in the Northern Hemisphere. Specific places where differences are at least as large as the estimated errors are: in
- the far north (46–53° N), GOSAT underestimates the seasonal cycle by 0.9 ppm. This latitudinal range is composed of 5 European sites and Park Falls. Park Falls underestimates the seasonal cycle by 0.4 ppm. This finding is consistent with Lindqvist et al. (2015). In 28–37° N (which consists only of Lamont), SCIAMACHY is 0.8 too large.





In the Southern Hemisphere (SH), CT2013b underestimates the seasonal cycle. Figure 10 shows a map of fits of the seasonal cycle amplitude of SCIAMACHY, GOSAT, CT2013b, and MACC with TCCON having at least 2 years of matches shown as circles. This map shows how the results of Table 4 fits into the global pattern (with the ⁵ model fields matched to GOSAT locations and times). Interestingly, the seasonal cycle amplitude varies longitudinally; this pattern is seen in both satellite datasets and both models. Since the amplitude is taken from the sampled harmonic there is no extrapolation although the seasonal cycle could be underpredicted at high latitudes where there are data gaps. This map is consistent with Lindqvist et al. (2015), Fig. 8 which also finds high values in the 45–50° N, 120–180° E range.

CO₂ yearly growth rate 4.2

10

The same fitting program in the above section, CCGCRV, also calculates a yearly increase. In Table 5 we compare the fitted yearly increase for TCCON to each of the datasets. Comparisons to TCCON are within the predicted error except the SH where SCIAMACHY is low compared to TCCON and in the 46-53°N range where GOSAT is low compared to TCCON. The yearly increase for TCCON varies from 1.9 to 2.3 ppm yr^{-1} for the different locations and time ranges. To see how much of the observed variability in the growth rate is temporal vs. spatial variability in the growth rate, we compare to the global annual increase (growth rate) from surface measure-

- ments (http://www.esrl.noaa.gov/gmd/ccgg/trends/global.html) shown in Table 6. The average global yearly increase predicted from Table 6 using the time periods in Table 5 are shown in the last column of Table 5. The correlation r value between "Yearly incr. TCCON" and "global" (Table 6) coloumns is 0.84 (similarly the correlation to Mauna Loa calculated average annual increase is 0.82), whereas the correlation r value between
- "Yearly incr. TCCON" and "Yearly incr." columns is 0.60. Therefore, the variability of the 25 seen in Table 5 is primarily explained by the time-range of the comparisons.

Reuter et al. (2011, JGR, Table 2) found agreement within the calculated errors at Park Falls and Darwin for BESD-SCIAMACHY and CT2009 vs. TCCON. However, older



datasets were used for this result. Looking specifically at Park Falls, we see 1.80 ± 0.14 and 2.10 ± 0.22 for SCIAMACHY and TCCON, respectively and at Darwin 1.67 ± 0.08 and 2.16 ± 0.05 for SCIAMACHY and TCCON, respectively, where the errors represent the standard deviation of SCIAMACHY fits for similar latitudes.

5 4.3 Seasonal cycle phase

25

This section looks at the time-offset correlation and standard deviation between the test datasets and TCCON. This checks whether, for example, a seasonal cycle is delayed or ahead of the TCCON seasonal cycle, which has important implications for flux estimates (Keppel-Aleks, 2012), whether there are seasonally dependent biases that are affecting the seasonal cycle, and whether the datasets are seeing the "same" seasonal cycle.

To compare seasonal cycle amplitudes, all datasets have 2 ppm yr^{-1} subtracted off to approximately remove secular increases (over the ± 60 days offset this has a very small effect). For a 0 day offset, the datasets are matched as usual. For a 1 day offset, TCCON is moved forward by 1 day and compared to the dataset. This is repeated for

TCCON is moved forward by 1 day and compared to the dataset. This is repeated for all offset times. Correlations are fit to a 2nd order polynomial to determine the phase minimum difference. As TCCON is moved forward or backward in time, different points will match up, particularly when there are data gaps in either dataset. This can cause difficulties in interpretation. The maximum correlation is limited by the ratio of the error to the variability. It follows from the definition of correlation that:

$$\operatorname{corr}_{max} = \operatorname{corr}_{o} \frac{1}{\sqrt{1 + (\varepsilon_{x}/\sigma_{x})^{2}} \sqrt{1 + (\varepsilon_{y}/\sigma_{y})^{2}}},$$

where corr_o is the noise-free correlation, ε_x is the error on x and σ_x is the true variability for x, ε_y is the error on y and σ_y is the true variability for y. Because we are estimating σ and ε , there is uncertainty on the correlation maximum. In our case σ_y is taken to be the TCCON variability and ε_y is estimated using Table 3 with 10 SCIAMACHY and



(3)

CC II

4 GOSAT averages. The error bars on the correlations are calculated from the fisher's *z* test. (Fisher, 1915, 1921). Figure 11 shows SCIAMACHY and GOSAT results at Park Falls. Although the prior performs well in regards to the standard deviation vs. TCCON Fig. 11 shows the prior has a clear seasonal cycle phase error which is corrected by the satellite retrievals for both SCIAMACHY and GOSAT at Park Falls.

Results of the seasonal cycle phase error are tabulated in Table 8, columns "GOSAT prior" and "GOSAT retrieved", "SCIA prior" and "SCIA retrieved". Stations not shown have either too few match-ups (e.g. Sodankyla) or too little variability compared to the noise (e.g. Wollongong) to have useful comparisons. The GOSAT retrieval markedly improves the appeared evelop phase variable and the seasonal evelop phase variable and the seasonal evelop phase variable.

- proves the seasonal cycle phase versus TCCON all stations where there is adequate data. The SCIAMACHY retrieval clearly improves over the prior for Park Falls and Four Corners, mildly improves in 3 and stays the same in 2 cases. Mismatches in SCIA-MACHY phase could be from mismatches in vertical sensitivity (as higher altitudes have lagged seasonal cycles), effects of coincidence criteria, or seasonal-dependent
- biases. To check the coincidence criteria, cross-correlations were done for the geometric coincidence criteria which had significantly fewer matchups. Similar results for geometric coincidence criteria were found for GOSAT and SCIAMACHY for Lamont and Park Falls; the other stations are too noisy to draw conclusions.

Table 7 also shows the phase differences for the models, which have closer spatial/temporal matches and lower single-matchup errors. Model-TCCON phase differences could result from errors in model flux distributions, seasonal timing, or transport errors. Table 7 shows the phase differences, which vary from -20 to +10 days. Phase differences more than 10 days are noticeable by eye and occur in the NH at: Bremen and Four Corners (negative) (these stations are influenced by local effects), and

Orleans and Izaña (positive, CT2013b only). Larger phase differences occur at some stations in the Southern Hemisphere. Although the seasonal cycle is weaker in the Southern Hemisphere, it can be clearly seen in, e.g. the Lauder_125HR data in Fig. 2. The correlations versus offset days show a phase difference of -20 days for CT2013b and +0 days for MACC at LAUDER_125HR, as seen in Fig. 12. Note that the fits of



the seasonal cycle in the SH display more complexity, such as multiple local maximum, than fits in the NH and "phase lag" could also be an indication of an issues with the fit shape. Figure 12 shows correlations and standard deviations versus day offset for 3 stations that have the seasonal cycle peak within \pm 10 days for CT2013b and MACC

- top panels), and for stations which have a larger phase lag compared to TCCON (bottom panels). There is often a small peak within ± 3 days, which indicates the models' capability of picking up variations that occur day to day (i.e., synoptic scale variability), which indicates the strength of synoptic activity and matching between models and TCCON. This peak is not seen in satellite data for dynamic coincidence criteria likely
- ¹⁰ due to matching, or geometric coincidence criteria likely due to the noise. Not that this synoptic peak occurs at 0 even when the seasonal cycle has a phase lag (e.g. MACC model at Bremen, in the lower right panel, or Lauder_125HR comparisons). The synoptic scale correlation varies between 0 and 0.17, as seen in Table 7.

A brief discussion on Izana. The TCCON station is on Tenerife Island, a small island (about 50 × 90 km) with complex topography located about 300 km west of southern Morroco. The TCCON station is located at 2.37 km (about 770 mb). The MACC and CT2013b models at ~ 2° × 3° resolution do not resolve topography at these scales and consequently have mean surface pressure at sea level, about 1000 hPa at this location. Our standard treatment is to interpolate the model to the TCCON pressure grid, then

- ²⁰ calculate X_{CO_2} using the TCCON pressure weighting function. At Izaña this has the effect of chopping off the lower atmosphere. The CT2013b result for this treatment has a ~ + 10 day seasonal cycle phase difference at Izaña; whereas MACC has no phase difference at Izaña. If, however, the model surface pressure is used to calculate X_{CO_2} , MACC goes from a 0 to a –10 day phase lag, and CT2013b has 0 phase difference. An
- argument for using the model surface pressure would be if the upslope winds at Izaña (Sancho et al., 1991; Bergamaschi et al., 2000) shifted the profile upwards rather than chopping it off, which would occur if the air instead deviated around the island. This finding has important implications on the choice of the comparison methodology and the ideal location for validation sites. Validation sites within complex geographical terrain





have to be treated as special cases as (a) the atmospheric models usually do not resolve these variations and (b) satellite measurements rarely have a perfect co-location with the ground-based site, meaning that they could sample a substantially different altitude level. This holds for both mountains (e.g. Izaña) and valleys (e.g. Garmisch).

⁵ This highlights one of the many choices that are made when comparing two products (e.g. whether to apply the averaging kernel, whether to use interpolation, how to treat the surface pressure, or what coincidence criteria to use).

Another finding worth noting is the comparisons at Lauder. In 2010 the Lauder125HR instrument began routine operation, while the Lauder 120HR instrument continued to take TCCON data up to through the end of 2010. Both MACC and CT2013b show no

- take TCCON data up to through the end of 2010. Both MACC and C12013b show no seasonal cycle correlation with the 120HR time series at Lauder, but do show correlation with Lauder125HR time series. We attribute this to the improved precision of the 125HR data, and an increase of the seasonal cycle amplitude in 2011 and 2012 as compared to other years (e.g. compare 2011 vs. 2007). The phasing error found in the CT2013b comparison with the Lauder 125HR may be due to CT2013b not modelling
- the drivers of the seasonal cycle amplification in 2011 and 2012.

At Bremen and Four Corners, local effects that do not affect CO_2 at 2 × 3° are likely dominating, particularly since Bremen is clustered with Orleans, Garmisch, and Karlsruhe, which all compare fine, and because the correlation of daily variability, as seen in the port section is also very low at these two stations

²⁰ in the next section, is also very low at these two stations.

5 Daily variability (models vs. TCCON)

At the surface, CO₂ shows a strong diurnal cycle in areas with active vegetation, e.g. Park Falls during summer, and synoptic trends based on regional dynamics. Even though the diurnal cycle is markedly smaller in the total column (Olsen and Randerson, 25 2004), it can be observed both by TCCON and also in models, in our case CT2013b and MACC, as seen in Fig. 13. Both diurnal variations and synoptic trends can be seen in Fig. 13. Validating the amplitude of the diurnal variability in the column is im-





portant as the column diurnal variability better represents the amount of CO₂ emitted or absorbed by surface processes as compared to surface measurements, which are impacted by boundary layer height. To our knowledge this is the first comparison of model fields to TCCON to compare the diurnal cycle. As TCCON itself has not been validated at multiple times in one day, this is considered a comparison not a validation.

- We compare the difference between morning and afternoon in models and TCCON. To minimize potential TCCON biases that depend on the solar zenith angle (through the air mass factor), we compare at two points in each day separated by the largest time with the same solar zenith angle (SZA). The methodology is to (1) identify two points,
- t_1 and t_2 , from the same day with the largest time difference but with the same SZA. As the TCCON data used in this paper has been averaged over 90 min, t_1 or t_2 may be interpolated between two time points. (2) We compare TCCON at t_2 minus TCCON at t_1 and the same times for each model. We look at the variability within one day for one season (JJA). Looking at different seasons for the Northern Hemisphere at the
- ¹⁵ bottom of Table 8, both models showed clearly higher correlations and slopes in MAM and JJA vs. DJF and SON. In the SH for other seasons, there was less consistency between model findings. For CT2013b, correlations were seen in MAM, JJA, and SON at Lauder-125HR, and JJA and SON at Darwin (0.3–0.7), but not the other seasons, and correlations only in SON at Wollongong (0.22). MACC did not show correlations with
 ²⁰ Darwin in any season, but showed the best correlations with Wollongong in JJA and
- SON (0.3–0.4), and correlations with Lauder-125HR in all seasons (0.24–0.6), peaking in DJF.

Table 8 show correlations between CT2013b or MACC vs. TCCON in the daily variability. The correlations are about 2/3 as large as could be expected, given the relative sizes of the variability and errors (see text around Eq. 3). When correlations are present the models have about 1/3 to 1/2 the variability of TCCON (as seen from the smaller slopes). In the far north (Ny Alesund, Sodanklya), the correlations indicate agreement but the model daily variability is less than 1/4 TCCON. In the mid-latitudes there is the highest correlation (~ 0.3–~ 0.7) with model daily variability ~ 0.2–0.6 that of TC-





CON. Bremen and Four Corners, the models do not show diurnal variability that is seen by TCCON. These are also the two stations in the mid-latitude NH which showed a seasonal cycle phase lag in both models. These sites are expected to be strongly influenced by local sources, a power plant for Four Corners, and urban sources for
 ⁵ Bremen. In the Southern Hemisphere, correlation is seen at Wollongong and Lauder

(125HR), again with less variability seen in models. Because of the smaller variability in the SH sites, the best correlation that could be achieved is about 0.3 for Darwin and Lauder120HR, 0.4 for Lauder125HR, and 0.5 for Darwin.

 The CT2013b model in general shows more daily variability and higher correlations,
 which are in better agreement with TCCON. Since the satellite observations are coincident ~ once per day, the diurnal pattern will not be constrained by satellite observations, except as preserved in transported air coincident with satellite measurements downwind. Model Observing System Simulation Experiments (OSSE) can determine the impact of the diurnal cycle strength on flux estimates to determine the importance
 of independently verifying the diurnal cycle in models.

6 Discussion and conclusions

We focus on validating aspects of model and satellite data which may be important for accurate flux estimates and CO₂ assimilation, including accurate error estimates, overall biases, biases by season and latitude, impact of coincidence criteria, validation of seasonal cycle phase and amplitude, yearly growth, and daily variability. The impact of our findings can be used for correcting data (e.g. Basu et al.,2013, accounted for global land/sea biases; Nassar et al., 2011, corrected for hemispheric gradients) or can be mitigated by assimilation method (e.g. the inversion method of Reuter et al., 2014, which is set up to be insensitive to seasonal and regional biases outside the investigated region). To determine the importance of the findings of this paper on flux

estimates, each type of bias found in this paper (seasonal biases, location-dependent biases, seasonal cycle differences, seasonal cycle phase differences, and diurnal cycle



differences) should be tested using an OSSE to determine its effect on flux biases and flux distribution errors. For example, Kulawik et al. (2013) tested the effect of a NH bias of 0.3–0.5 ppm in JJA, finding flux biases comparable to GOSAT updates in some regions.

- ⁵ We find standard deviations of 0.9, 0.9, 1.7, and 2.1 ppm versus TCCON for CarbonTracker, MACC, GOSAT, and SCIAMACHY, respectively. GOSAT predicted error should be multiplied by 1.9 and SCIAMACHY predicted error should be multiplied by 0.9 to represent the actual single target error. There is a correlation *r* value of 0.5 for SCIAMACHY and 0.6 for GOSAT for the actual and predicted errors grouped by sta-
- ¹⁰ tion. Equation (2) and Table 3 show how errors decrease when satellite results are averaged and estimate the magnitude of the correlated and random errors components for averaged satellite results, where random error components decrease with increasing number of averaged observations. When satellite data are averaged and interpreted according to the model error² = $a^2 + b^2/n$ (where *n* are the number of observations averaged, *a* are the systematic (correlated) errors, and *b* are the ran-
- ¹⁵ observations averaged, *a* are the systematic (correlated) errors, and *b* are the random (uncorrelated) errors), $a = 0.6 \pm 0.3$ ppm and $b = 1.7 \pm 0.3$ ppm for GOSAT, and $a = 1.0 \pm 0.3$ ppm, $b = 1.4 \pm 0.4$ ppm for SCIAMACHY regional averages (dynamic coincidence criteria) in the Northern Hemisphere, correcting for coincidence errors and TCCON errors. SCIAMACHY averaging results in the lowest correlated errors when
- ²⁰ using dynamic coincidence criteria where values are averaged from a larger spatiotemporal region, whereas GOSAT, in the two stations where sufficient data exists (Lamont, Park Falls), geometric criteria performs better than dynamic coincidence criteria. These data represent averaging of satellite data which matches a single TCCON value. The above error model should help assigning realistic retrieval error correlations in as-
- similation systems in place of current ad hoc hypotheses (see, e.g., Sect. 2.2 in Basu et al., 2013, for an example of such hypotheses).

Biases vary by station (see Fig. 3); the station-dependent biases have a standard deviation of ~ 0.3 ppm from year to year. Biases larger than ~ 0.3 ppm likely represent persistent biases. Biases of this magnitude are seen in many stations for all datasets,





particularly Eureka, Ny Alesund, Sodankyla in the far north, Garmisch, Four Corners, JPL (MACC only), Tsukuba (satellites only), and Lauder (satellites only). Biases also vary by time. Looking seasonally, and subtracting the overall bias, there are also persistent biases affecting the seasonal cycle amplitudes on the order of -0.8 to 0.8 ppm.

- ⁵ However, note that the TCCON bias uncertainty is on the order of 0.4 ppm; the TCCON team is working to improve this. The persistent seasonal biases were that SCIAMACHY for 0–45° N is high in MAM, low in JJA, on the order of 1.2 ppm total spread; poleward of 45° N GOSAT and SCIAMACHY are low in DJF and high in JJA on the order of 0.3–0.5 ppm, and MACC is high in DJF and low in SON on the order of 0.3 ppm.
- Related to the seasonal biases, we validate the seasonal cycle amplitudes, which are important for biospheric flux attribution. All sets show the same general patterns for the different latitude bands (SH, 28–37° N, 46–53° N, 67–79° N). The discrepancies versus TCCON which are statistically significant are that GOSAT has too small a seasonal amplitude in the 46–53° N range by 0.9 ppm, SCIAMACHY overestimates 28–37° N (which includes only Lamont) by 0.8 ppm, and CT2013b is too small in the SH by 0.5 ppm. A
- preliminary study of how a seasonal bias in JJA in GOSAT of 0.5 ppm in the NH would affect fluxes using a global assimilation showed that the effect was not minor (Kulawik et al., 2013).

The seasonal cycle phase can detect seasonally dependent biases in satellite data and issues with model fluxes or transport errors. We investigate the alignment of the seasonal cycles by offsetting each CO₂ set versus TCCON by -60 to + 60 days. For satellites, the following stations had adequate data and high enough signal/error to estimate a result: Bialstok, Karlsruhe, Orleans, Garmisch, Park Falls, Four Corners, Lamont, and Izaña (GOSAT only). The GOSAT r.m.s. phase difference versus TCCON is

²⁵ 16.9 days for the prior and 4.7 days for the GOSAT retrieved X_{CO_2} , a marked improvement. SCIAMACHY improved substantially at 2 of 7 sites, and SCIAMACHY r.m.s. phase difference versus TCCON is 16.3 days for the prior and improves to 13.4 days for the SCIAMACHY retrieved X_{CO_2} . Model comparisons to TCCON are much less noisy as there are many more matches. Most NH stations show the expected seasonal



dropoff (e.g. see Fig. 12), with the peak correlation near 0 days, and an additional spike within ± 3 days indicating the capture of synoptic variability. Stations that showed phase differences larger than 10 days are Four Corners (both models), Bremen (both models), Izana (CT2013b only), Darwin (Macc only), and Lauder 125HR (CT2013b 5 only).

In studying the variability through a single day, both models show correlation to the variability within a day versus TCCON, on the order of 0.2–0.8 correlation for NH stations, about 2/3 of the possible correlation given the errors (except at Bremen and Four Corners which had little correlation and no slope). The amplitude of the variability is higher in TCCON versus the models with CT2013b closer to TCCON than MACC

- ¹⁰ is higher in TCCON versus the models, with CT2013b closer to TCCON than MACC. However, TCCON daily variability has not been validated (there are plans to validate TCCON throughout the day in the near future). Diurnal pattern will not be constrained by satellite observations, except as preserved in transported air coincident with satellite measurements downwind, and therefore may be important to independently verify the diversel avelage to except a security approximate activity of the security of t
- diurnal cycle in models to ensure accurate satellite assimilation results. The importance of the diurnal cycle on flux estimates would need to be tested.

In our analysis a clear picture has emerged of two TCCON stations (Bremen, Four Corners) most influenced by local sources, seen in phase differences versus models, daily variability, and large overall biases. Caution should be used when using these

- stations for validation. Spatial and seasonal-dependent biases are obstacles to accurate and better resolved CO₂ flux estimates. This paper highlights findings that provide inputs to estimate flux errors in model assimilations, and places where models and satellites need additional validation or improvement. Some of the issues which need further investigation are: the GOSAT seasonal cycle in 46–53° N latitude range (which
- is 0.9 ppm smaller than TCCON), SCIAMACHY over-predicting the seasonal cycle at Lamont, both models with seasonal cycle differences at the different SH stations, differences in the diurnal cycle amplitude between models and TCCON, and high biases for GOSAT and SCIAMACHY north of 67° N.





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Table 1. Summary of the CO_2 datasets and models we are using showing the coverage for several different CO_2 products. The obs/day are the approximate number of CO_2 observations which pass quality screening.

| Satellite/TCCON | Dates available | day/ night | land/ ocn | latitude | obs/ day | footprint |
|--|--|-------------------|----------------------|---|---------------------|---------------------------------|
| SCIAMACHY v2.00.08 GOSAT ACOS-v3.5 TCCON GGG2012 | Jan 2003–Apr 2012 Jun 2009–Apr 2014 see Fig. 1 | day day day | land both both | 80° S–80° N 80° S–80° N 45° S–80° N | ~ 800 ~ 360 - | 60 × 30 km 10.5 km cir. – |
| Model | Dates available | | | Time res. | Spatial | res. (lat × lon) |
| CT2013b MACC 13.1 | 2000–2012 1979–2013 (used 20 | 07–201 | 3) | 3 h 3 h | 2 × 3° (1.9 × 3 | global, 1 × 1° US .75° |

 Table 2. Coincidence criteria, data versions, and terminology used in our analysis.

| Coincidence criteria | |
|------------------------|--|
| Geometric Dynamical | 5° in lat/lon, ± 1 h from Wunch et al. (2011). Considers free-tropospheric temperature, $\pm 10^{\circ}$ lat, $\pm 30^{\circ}$ lon and 5 days (see Sect. 3.1) |
| Datasets | |
| GOSAT | ACOS-GOSAT version 3.5 with corrections and quality flags from the user's guide |
| SCIAMACHY | BESD-SCIAMACHY v02.00.08 |
| TCCON | GGG2014 when available, GGG2012 data from Four Corners, Tsukuba, and Bremen with GGG2012 bias corrections applied as described in Sect. 2.3 |
| CarbonTracker | CT2013b |
| MACC | MACC v13.1 |
| | |

Averaging: All averaging is done by station first and then averaging over station results.

Model choices: MACC is interpolated to TCCON latitude, longitude, and time. CT2013b special output is interpolated to TCCON time. Model XCO₂ uses TCCON surface pressure.





Table 3. Fit of *a* and *b* in Eq. (2), with stations having data out to at least n = 50 for dynamic coincidence criteria, n = 20 (GOSAT) or n = 40 (SCIAMACHY) for geometric coincidence criteria. The CT-CT column describes the standard deviation of CT@satellite vs. CT@TCCON at the largest *n* for that station, providing a lower bound on the satellite/TCCON differences. The "subtr co-location error" row estimates the correlated error for satellites only, subtracting in quadrature TCCON error (0.44 ppm) and co-location error (0.3 or 0.7 ppm). The GOSAT geometric averages are $a = 0.7 \pm 0.1$, $b = 1.5 \pm 0.1$, a "subtr co-location error" = 0.5 ± 0.1 .

| | Geometric | | Dynamic | | | Dynamic/Geometric | | | |
|-------------------|---------------|---------------|---------------|---------------|---------------|-------------------|---------------|---------------|---------------|
| | SCIAN | 1ACHY | CT-CT | SCIAN | IACHY | CT-CT | GO | SAT | CT-CT |
| Station | а | b | а | a | b | а | а | b | а |
| Bialystok | 1.7 | 1.5 | 0.2 | 1.2 | 2.1 | 0.8 | 0.8 | 1.8 | 0.8 |
| Bremen* | 1.1 | 1.6 | 0.2 | 1.3 | 2.0 | 0.7 | 1.6 | 1.8 | 0.7 |
| Karlsruhe | 1.6 | 1.9 | 0.4 | 1.3 | 1.1 | 0.8 | 1.0 | 18 | 0.9 |
| Orleans | 1.5 | 1.7 | 0.2 | 1.1 | 1.2 | 0.5 | 0.9 | 1.9 | 0.4 |
| Garmisch | 1.9 | 1.4 | 0.7 | 1.3 | 1.1 | 1.0 | 0.9 | 1.9 | 1.0 |
| Park Falls | 1.2 | 1.6 | 0.2 | 1.2 | 1.5 | 0.8 | 1.1/0.7 | 1.8/1.5 | 0.8/0.3 |
| Lamont | 1.2 | 1.5 | 0.3 | 1.2 | 2.0 | 0.6 | 1.1./0.8 | 1.6/1.4 | 0.6/0.3 |
| Izaña | - | - | - | 0.7 | 1.1 | 0.4 | 0.6 | 1.3 | 0.4 |
| Mean NH | 1.5 ± 0.3 | 1.6 ± 0.2 | 0.3 ± 0.2 | 1.1 ± 0.2 | 1.4 ± 0.4 | 0.7 ± 0.2 | 0.9±0.2 | 1.7 ± 0.3 | 0.7 ± 0.2 |
| Mean NH: subtr | 1.4 ± 0.4 | - | _ | 1.0 ± 0.3 | _ | _ | 0.6 ± 0.3 | - | _ |
| co-location error | | | | | | | | | |
| Darwin | 1.4 | 1.5 | 0.1 | 1.3 | 1.2 | 0.1 | 0.7 | 1.1 | 0.2 |
| Wollongong | 1.0 | 1.8 | 0.2 | 1.2 | 1.8 | 0.2 | 0.8 | 1.3 | 0.2 |
| Mean SH | 1.2 ± 0.3 | 1.6 ± 0.2 | 0.2 ± 0.1 | 1.3 ± 0.1 | 1.5 ± 0.4 | 0.2 ± 0.1 | 0.8±0.1 | 1.2 ± 0.1 | 0.2 ± 0.0 |

* Bremen is influenced by local effects and is not included in averages.



Table 4. Seasonal cycle amplitudes. Each comparison to TCCON uses a time period based on the available matchups (see Table 1), stations, observations which have at least 2 years of data for comparisons. Stations included for satellites are: Bialystok, Bremen, Karlsruhe (GOSAT), Orleans, Garmisch, Park Falls, Four Corners (GOSAT), Lamont, Izaña (Gosat), Darwin, and Wollongong. Stations included for satellites are: Bialystok, Bremen, Karlsruhe (GOSAT), Orleans, Garmisch, Park Falls, Four Corners (GOSAT), Lamont, Izaña (GOSAT), Darwin (GOSAT), Orleans, Garmisch, Park Falls, Four Corners (GOSAT), Lamont, Izaña (GOSAT), Darwin (GOSAT), and Wollongong, Lauder_120HR, and Lauder_125HR. Bold shows entries with differences larger than the predicted error which is the greater of: the bootstrap error (Rubin, 1981) (on the order of 0.1 ppm), variability within the latitude bin (the dominant error).

| Comparison | Region | Seasonal amp. (ppm) | Seasonal amp. TCCON (ppm) | Seasonal amp. difference ppm) |
|------------|--------------------------|---------------------------------|---------------------------------|-------------------------------------|
| CT2013b | 67–79° N (<i>n</i> = 2) | 10.1 ± 0.1 | 10.0 ± 0.5 | 0.1 ± 0.6 |
| | 46–53° N (<i>n</i> = 4) | 7.6 ± 0.3 | 7.9 ± 0.4 | -0.4 ± 0.5 |
| | 28–37° N (<i>n</i> = 2) | 4.7 ± 0.9 | 5.5 ± 0.5 | 0.8 ± 1.0 |
| | SH (<i>n</i> = 4) | $\textbf{0.9} \pm \textbf{0.3}$ | $\textbf{1.4} \pm \textbf{0.4}$ | $-~0.5\pm0.5$ |
| MACC | 67–79° N (<i>n</i> = 3) | 11.0 ± 0.3 | 10.7 ± 0.3 | 0.3 ± 0.4 |
| | 46–53° N (<i>n</i> = 4) | 8.2 ± 0.3 | 8.0 ± 0.5 | 0.1 ± 0.6 |
| | 28–37° N (<i>n</i> = 2) | 5.5 ± 0.1 | 5.4 ± 0.4 | 0.1 ± 0.3 |
| | SH (<i>n</i> = 4) | 1.1 ± 0.3 | 1.3 ± 0.1 | -0.2 ± 0.4 |
| GOSAT | 46–53° N (<i>n</i> = 6) | $\textbf{7.2} \pm \textbf{0.5}$ | $\textbf{8.1} \pm \textbf{0.4}$ | $-\ 0.9\pm0.6$ |
| (v3.5) | 28–37° N (<i>n</i> = 3) | 5.3 ± 0.3 | 5.1 ± 0.1 | 0.2 ± 0.3 |
| | SH (<i>n</i> = 2) | 1.6 ± 0.5 | 1.8 ± 0.8 | -0.2 ± 0.9 |
| SCIAMACHY | 46–53° N (<i>n</i> = 4) | 7.7 ± 0.5 | 7.4 ± 0.9 | 0.3 ± 1.2 |
| (BESD- | 28–37° N (<i>n</i> = 1) | 7.2 ± 0.1 | $\textbf{6.4} \pm \textbf{0.1}$ | $\textbf{0.8} \pm \textbf{0.2}$ |
| v02.00.08) | SH (<i>n</i> = 1) | 2.6 ± 0.3 | 1.8 ± 0.7 | 0.8 ± 0.8 |





Table 5. Yearly increases. Each comparison uses matched pairs with TCCON using locations which have at least 2 years of data for comparisons. See Table 4 for stations included. The start date and end date are averaged for the stations in each bin and are shown in the next to last column. Bold text shows one difference larger than predicted errors. The last column shows the average global yearly increase for the time period using Table 6.

| | | | Yearly incr. | Yearly incr. | | global |
|------------|--------------------------|-----------------------------------|-----------------------------------|-----------------|---------------|-------------------------|
| | | Yearly incr. | TCCON | Difference | Period | (Table 6) |
| Comparison | Region | (ppm yr ⁻¹) | (ppm yr ⁻¹) | $(ppm yr^{-1})$ | (year fract) | (ppm yr ⁻¹) |
| CT2013b | 67–79° N (<i>n</i> = 2) | 2.05 ± 0.23 | 2.03 ± 0.21 | 0.0 ± 0.3 | 2007.7-2012.8 | 1.99 |
| | 46–53° N (<i>n</i> = 6) | 2.11 ± 0.09 | 2.12 ± 0.12 | -0.0 ± 0.2 | 2008.1-2013.1 | 2.02 |
| | 28–37° N (<i>n</i> = 2) | 2.05 ± 0.07 | 2.00 ± 0.09 | -0.0 ± 0.1 | 2007.9-2013.1 | 2.01 |
| | SH (<i>n</i> = 4) | 1.96 ± 0.04 | 1.98 ± 0.20 | 0.0 ± 0.1 | 2007.7–2012.6 | 1.97 |
| MACC | 67–79° N (<i>n</i> = 2) | 2.10 ± 0.17 | 2.20 ± 0.06 | 0.1 ± 0.2 | 2009.1-2013.4 | 2.11 |
| v13.1 | 46–53° N (<i>n</i> = 6) | 2.22 ± 0.10 | 2.21 ± 0.11 | 0.0 ± 0.1 | 2008.5-2013.9 | 2.11 |
| | 28–37° N (<i>n</i> = 2) | 2.20 ± 0.04 | 2.08 ± 0.12 | 0.1 ± 0.1 | 2008.0-2013.9 | 2.08 |
| | SH (<i>n</i> = 4) | 2.10 ± 0.08 | 2.08 ± 0.06 | 0.0 ± 0.1 | 2008.0-2013.9 | 2.08 |
| GOSAT | 46–53° N (<i>n</i> = 6) | $\textbf{2.04} \pm \textbf{0.02}$ | $\textbf{2.27} \pm \textbf{0.06}$ | -0.2 ± 0.1 | 2009.4-2013.9 | 2.11 |
| v3.5 | 28–37° N (<i>n</i> = 2) | 2.24 ± 0.02 | 2.29 ± 0.20 | -0.0 ± 0.2 | 2009.3–2013.9 | 2.20 |
| | SH (<i>n</i> = 3) | 2.10 ± 0.03 | 2.10 ± 0.09 | 0.0 ± 0.1 | 2009.4–2012.9 | 2.23 |
| SCIAMACHY | 46–53° N (<i>n</i> = 5) | 2.00 ± 0.15 | 1.99 ± 0.07 | 0.0 ± 0.1 | 2007.8-2012.2 | 1.93 |
| BESD-V2 | 28–37° N (<i>n</i> = 1) | 2.11 ± 0.14 | 2.15 ± 0.22 | -0.0 ± 0.3 | 2008.5-2012.2 | 1.92 |
| | SH (<i>n</i> = 1) | $\textbf{1.79} \pm \textbf{0.09}$ | $\textbf{1.94} \pm \textbf{0.05}$ | -0.1 ± 0.1 | 2008.5-2012.2 | 1.92 |



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Table 6. Annual increase globally and at Mauna Loa from ESRL website (http://www.esrl.noaa. gov/gmd/ccgg/trends/global.html).

| Year | Global (ppm yr ⁻¹) | Mauna Loa (ppm yr^{-1}) |
|------|--------------------------------|----------------------------|
| 2006 | 1.74 ± 0.06 | 1.76 ± 0.11 |
| 2007 | 2.10 ± 0.07 | 2.22 ± 0.11 |
| 2008 | 1.78 ± 0.05 | 1.60 ± 0.11 |
| 2009 | 1.65 ± 0.10 | 1.88 ± 0.11 |
| 2010 | 2.44 ± 0.06 | 2.45 ± 0.11 |
| 2011 | 1.71 ± 0.09 | 1.84 ± 0.11 |
| 2012 | 2.43 ± 0.09 | 2.66 ± 0.11 |
| 2013 | 2.53 ± 0.09 | 2.05 ± 0.11 |
| 2014 | 1.86 ± 0.09 | 2.13 ± 0.11 |

Table 7. The left two numerical columns show standard deviation drop within ± 2 days of zero offset. Higher values indicate sites where temporal co-location is more important. The next two numerical columns show calculated phase difference between CT2013b, MACC and TCCON in days. A phase difference of -10 days means that the model seasonal cycle is 10 days behind TCCON. The next 4 columns show the same calculations for SCIAMACHY and GOSAT prior and retrieved values. Blank values are those for which a good fit was not found.

| | synop | otic | phase difference (days) | | | | | |
|---------------|---------|-------|-------------------------|------|-------|-----------|-------|-----------|
| Station | CT2013b | MACC | CT2013b | MACC | SCIA | SCIA | GOSAT | GOSAT |
| | (ppm) | (ppm) | | | prior | retrieved | prior | retrieved |
| Eureka | 0.1 | 0.0 | +5 | 3 | | | | |
| Ny Alesund | 0.2 | 0.2 | +1 | -2 | | | | |
| Sodankyla | 0.3 | 0.3 | -4 | -5 | | | | |
| Bialstok | 0.4 | 0.2 | +4 | +4 | 19 | 18 | 18 | 6 |
| Bremen* | 0.2 | 0.2 | -12 | -16 | | | | |
| Karlsruhe | 0.5 | 0.3 | 1 | -3 | 14 | 11 | 17 | 3 |
| Orleans | 0.4 | 0.3 | +8 | -1 | 11 | 11 | 3 | -3 |
| Garmisch | 0.4 | 0.3 | -7 | -7 | 9 | 8 | 11 | 2 |
| Park Falls | 0.5 | 0.3 | -2 | -5 | 13 | -1 | 18 | 3 |
| Four Corners* | 0.1 | 0.1 | -11 | -10 | -22 | -16 | -15 | -9 |
| Lamont | 0.5 | 0.3 | -7 | -5 | -14 | -14 | -9 | -2 |
| Tsukuba | 0.4 | 0.2 | +5 | +2 | | | | |
| JPL2007* | 0.1 | 0.0 | +1 | -2 | | | | |
| Izaña | 0.0 | 0.0 | +10 | -4 | | | -25 | 0 |
| Darwin | 0.0 | 0.1 | +5 | -17 | | | | |
| Wollongong | 0.1 | 0.07 | | +8 | | | | |
| Lauder_125HR | 0.1 | 0.1 | -20 | +0 | | | | |

* Sites expected to be strongly influenced by local sources.

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Table 8. Diurnal variability of CT2013b and MACC13.1 versus TCCON in JJA arranged by latitude. TCCON variability and maximum theoretical correlation are shown, as well as actual correlation and slope for both models. The slope is the mode vs. TCCON fit to a straight line. Max corr. is calculated using Eq.(3), TCCON stdev, and the lower of the model-TCCON standard deviations from Appendix A. TCCON range, std shows the range of the values seen for the daily variability for TCCON, as well as the standard deviation of the TCCON daily differences. The Average row is for all entries above it. The AverageDJF, etc., rows are for stations Karlsruhe, Orleans, Garmisch, Park Falls, and Lamont.

| Station | Lat (°) | тсс | ON | Max Corr. | CT2013b | | MACC 13.1 | |
|--|--------------|---------------------|-------------|-----------|-------------|-------|-------------|-------|
| | | range (ppm) | stdev (ppm) | (Eq. 3) | Correlation | Slope | Correlation | Slope |
| Nyalesund | 79 | -2 to +2 | 0.6 | 0.6 | 0.22 | 0.14 | 0.27 | 0.04 |
| Sodanklya | 67 | -1.5 to +1.5 | 0.5 | 0.6 | 0.63 | 0.32 | 0.40 | 0.19 |
| Bialystok | 53 | -2 to +1 | 0.5 | 0.6 | 0.59 | 0.60 | 0.64 | 0.35 |
| Bremen* | 53 | -2 to +1 | 0.7 | 0.5 | 0.48 | 0.09 | -0.02 | 0.00 |
| Karlsruhe | 49 | -2 to 0 | 0.7 | 0.6 | 0.58 | 1.04 | 0.62 | 0.56 |
| Orleans | 48 | -1 to +0.5 | 0.7 | 0.7 | 0.75 | 0.43 | 0.70 | 0.31 |
| Garmisch | 47 | -3 to 0 | 0.8 | 0.6 | 0.58 | 0.56 | 0.69 | 0.46 |
| Park Falls | 46 | -3.5 to +2 | 1.0 | 0.8 | 0.77 | 0.32 | 0.54 | 0.23 |
| Four Corners* | 37 | -4.5 to +0.5 | 1.8 | 0.9 | 0.85 | 0.04 | 0.22 | 0.02 |
| Lamont | 37 | -3.0 to +1.0 | 0.8 | 0.7 | 0.70 | 0.23 | 0.32 | 0.14 |
| Tsukuba | 36 | -2 to +1.5 | 0.8 | 0.6 | 0.59 | 0.58 | 0.64 | 0.24 |
| Izaña | 28 | -0.5 to +0.5 | 0.1 | 0.2 | 0.20 | 0.16 | 0.45 | 0.04 |
| Darwin | -12 | -0.5 to +0.5 | 0.2 | 0.3 | 0.27 | 0.02 | 0.10 | 0.03 |
| Wollongong | -34 | -1.5 to +1.0 | 0.4 | 0.5 | 0.48 | 0.18 | 0.26 | 0.14 |
| Lauder120HR | -45 | -0.5 to +0.5 | 0.3 | 0.3 | 0.34 | 0.02 | 0.20 | 0.02 |
| Lauder125HR | -45 | -0.5 to +0.5 | 0.2 | 0.4 | 0.44 | 0.51 | 0.31 | 0.06 |
| Average JJA fo | r all statio | ons | | 0.6 | 0.44 | 0.33 | 0.40 | 0.18 |
| Average DJF (see caption for station list) | | | 0.6 | 0.36 | 0.15 | 0.33 | 0.08 | |
| Average MAM (see caption for station list) | | | | 0.6 | 0.54 | 0.35 | 0.51 | 0.23 |
| Average JJA (s | ee captic | on for station list | :) | 0.6 | 0.45 | 0.46 | 0.52 | 0.29 |
| Average SON (| see capti | ion for station lis | st) | 0.6 | 0.39 | 0.22 | 0.22 | 0.09 |

* Sites expected to be strongly influenced by local sources.





Table A1. We estimate the 90-min average TCCON standard deviation error by calculating the standard deviation (SD) of adjacent time points and model standard deviation of CT2013b and MACC13.1 versus TCCON by station. These values are used to estimate theoretical maximum correlations for seasonal cycle and diurnal correlations using Eq. (3).

| Station | TCCON adjacent SD (ppm) | CT2013b SD (ppm) | MACC SD (ppm) |
|---------------------------|----------------------------|---------------------|------------------|
| Eureka | 0.2 | 0.8 | 0.9 |
| Ny Alesund | 0.8 | 0.8 | 0.8 |
| Sodankyla | 0.3 | 0.7 | 0.8 |
| Bialystok | 0.3 | 0.7 | 0.7 |
| Bremen ^a | 0.5 | 1.3 | 1.4 |
| Karlsruhe | 0.4 | 0.9 | 0.9 |
| Orleans | 0.3 | 0.7 | 0.7 |
| Garmisch | 0.3 | 0.9 | 0.9 |
| Park Falls | 0.4 | 0.8 | 0.8 |
| Four Corners ^a | 0.7 | 1.1 | 1.1 |
| Lamont | 0.3 | 0.8 | 0.8 |
| Tsukuba ^b | 0.9 | 1.0 | 1.1 |
| JPL2007 ^a | 0.6 | 1.3 | 1.1 |
| Izaña | 0.2 | 0.8 | 0.6 |
| NH average | 0.44 | 0.91 | 0.92 |
| NH average (subset) | 0.35 | 0.79 | 0.79 |
| Darwin | 0.4 | 0.9 | 1.0 |
| Wollongong | 0.4 | 0.8 | 0.7 |
| Lauder | 0.4 | 0.8 | 0.8 |
| Lauder125 | 0.3 | 0.6 | 0.5 |
| SH average | 0.38 | 0.78 | 0.75 |

^a Stations strongly influenced by local effects; ^b higher TCCON error. These stations have been removed in the "NH average (subset)" row.

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Figure 1. TCCON site locations used for this work. The color indicates the year when each station started collecting data.















Figure 3. Bias (left) and standard deviation (right) for CT2013b, MACC, BESD-SCIAMACHY, and ACOS-GOSAT versus TCCON stations, arranged from high to low latitude. Comparisons which have a particularly low number of matches are TSUKUBA and LAUDER for SCIAMACHY and LAUDER for GOSAT.







Figure 4. Overall bias (left, with error bars showing the standard deviation of the bias) and standard deviation (right, with stars showing the predicted error for satellites) for most stations (some stations removed, see text).





Figure 5. SCIAMACHY and GOSAT standard deviation versus TCCON for different coincidence criteria and # of satellite observations averaged, n, in the Northern Hemisphere. The following consistent set of stations was used for all comparisons: Bialystok, Bremen, Karlsruhe, Orleans, Garmisch, Park Falls, Lamont, Darwin, and Wollongong. The dotted line shows the error if it scaled as the inverse square root of the number of averaged observations. The far right case for each of the categories contains the maximum n that has results for all stations.





Figure 6. Averaging matches of satellite data versus TCCON at Lamont. As the number averaged increases, the standard deviation versus TCCON decreases. CT2013b at the satellite versus at CT2013b at TCCON (purple) is used to quantitate spatio-temporal mismatch error. The points are fit to Eq. (2) (black). For GOSAT the uncorrected data is also fit (black dashed). We see that in this case, for GOSAT at Lamont, averaging more than about 4 observations improves over the initial guess.







Figure 7. Bias for 3 month groups for each station, where each station is normalized to have 0 yearly bias. For satellites, stations are included when at least 20 matches are found in each season. Dynamic coincidence criteria are used. The station colors are coded by location: far NH gray, European read/yellow, mid-latitude green, SH blue.







Figure 8. Bias for 3 month groups for Southern Hemisphere (left), 0–45° N (middle), and poleward of 45° N (right). Each group is normalized to have zero average over the year. The Southern Hemisphere (left, Lauder (except SCIAMACHY), Wollongong, and Darwin) has relatively small biases. The results that are significant are that for 0–45° N (Lamont, Tsukuba, Izana), SCIAMACHY is high for MAM, low for JJA; for > 45° N (Bialystok, Karlsruhe, Orleans, Garmisch, Park Falls, Eureka (models), Ny Alesund (models), and Sodankyla (models)), MACC is high, and GOSAT and SCIAMACHY are low in DFJ; GOSAT and SCIAMACHY are high in JJA (reducing the seasonal cycle).







Figure 9. Time series of matches at Park Falls, WI, USA using the dynamic criteria for TCCON and GOSAT with fits by the NOAA CCGCRV program.







Figure 10. Seasonal Cycle amplitude. The TCCON values are shown in the circles. The averaging is done over $10 \times 10^{\circ}$ bins every 5°. Comparisons vs. TCCON may be different than Table 4, since Table 4 has very close criteria for models and dynamic coincidence criteria for satellite data. The models are sampled at GOSAT observations.







Figure 11. Top: Cross correlation between TCCON and SCIAMACHY (top, left) and GOSAT (top, right) with matches using dynamic criteria at Park Falls. The *x* axis shows results when satellite data is offset in days versus TCCON. The dashed line shows the expected maximum correlation based on the error (see Eqs. 2, 3). The gray line is the correlation for the satellite priors, which are each out of phase by at least > 10 days. The * is the peak of a polynomial fit of the correlation between -25 and +25 days. Bottom: standard deviation between TCCON and SCIAMACHY (bottom, left) and GOSAT (bottom, right). The dashed line shows the Eq. (2) predicted error.







Figure 12. Top: Cross correlation examples between TCCON and CT2013b (left) or MACC (right). Each panel shows the correlation and 2nd order polynomial fits (top) and standard deviation (bottom) versus offset in days of TCCON versus satellite data. The correlation should be at a maximum and standard deviation at a minimum at days offset = 0. The top panels shows examples of stations in with phase less than 10 days. The bottom set shows example stations which have phase differences of at least 10 days for one or both of the models.







Figure 13. (a) Time series for models and TCCON from 1–8 August 2011 at Bialystok. The end-points of the solid lines show the time points used for comparing daily variability; both diurnal and synoptic variations are seen. **(b)** Change throughout the day at Bialystok for 2 August 2011. The large diamonds at 6 a.m. and 6 p.m. show the two times with largest difference that have the same solar zenith angle that are used in the analysis. The difference between these times are -2, -1.7, and -0.7 ppm for TCCON, CT2013b, and MACC, respectively. Right: CarbonTracker **(c)** and MACC **(d)** daily trends versus TCCON daily trends for BIALYSTOK in JJA, from compiling differences like shown in **(b)**. Correlation is seen in the daily trends as compared to TCCON with the daily amplitude for the models smaller than TCCON.



