Supplementary Material for Interpreting Seasonal Changes in the Carbon Balance of Southern Amazonia Using Measurements of XCO₂ and Chlorophyll Fluorescence from GOSAT

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Supplementary material for this letter contains information on satellite retrievals of total column CO₂ (XCO₂) and solar induced chlorophyll fluorescence (SIF) from
GOSAT, and methods describing the calculation of gross primary production (GPP). We start with a discussion of the ACOS b2.9, ACOS b2.10, RemoTeC, and NIES retrieval products, including pre- and post-processing procedures and bias correction techniques, and comparison of XCO₂ retrieval algorithms (Text S1). A description of SIF, including an estimate of GPP from SIF, is included in Text S2. Correlation and slope between XCO₂ and SIF for different retrieval products are shown in Text S3. We also discuss biomass burning as another source of XCO₂ later in the dry season of 2010 (Text S4).

**Text S1. XCO₂**

**A. Data Screening and Bias Correction**

Much care is taken to limit retrievals to those in which we have the highest confidence, and discard retrievals contaminated by clouds and other known error sources. For ACOS b2.9, we follow the procedure outlined in the ACOS Level 2 Data User’s Guide [Osterman et al., 2011], including a “master quality flag,” additional post-processing filters described in Table 3 of the User’s Guide, and a cloud flag. For ACOS b2.10, which has not been released publicly, we follow a similar procedure, with slight modifications to filtering criteria (chi2_o2 < 1.25, chi2_weak < 1.6, chi2_strong < 2, aod_total < 0.15, -1000 < dp < 700 pa, diverged <= 2, and blended albedo < 0.8). Screening procedures for RemoTeC is described in Butz et al. [2011]. Pre- and post-screening criteria for NIES is described in the following document available via internet (https://data.gosat.nies.go.jp/GosatWebDds/productorder/distribution/user/V02xx_FTS_S WIRL2_ReleaseNote_GU_en.pdf). The accuracy of ocean glint retrievals is still under investigation [Wunch et al., 2011; Crisp et al., 2012; O’Dell et al., 2012] and therefore glint data is ignored in this study.
Although the pre- and post-processing steps are unique to each retrieval product, in all cases a significant amount of soundings are removed over the Amazon due to cloud contamination and high aerosol loads (see Fig. S1, where the blue box indicates region 1 discussed in the main text and the red box region 2). In particular we note that 90% or more of soundings are removed in the central Amazon such that several averaging bins don’t fully resolve the seasonal cycle. Post-processed and detrended XCO$_2$ retrievals, averaged over the Amazon Basin, are shown in Fig. S2.

Fig. S1. Number of XCO$_2$ retrievals over Amazon from ACOS b2.9 (top right), ACOS b2.10 (top right), RemoTeC (bottom left) and NIES (bottom right) from July 2009.
through December 2010, aggregated over 2.5°x2° grid boxes. Amazonia boundary is demarcated by the black line and regions 1 and 2 by blue and red boxes, respectively.

Errors in the XCO$_2$ retrievals have been found to correlate well with certain other retrieved variables at regional scale such as surface albedo, surface pressure, air masses, and A-band signal levels. This issue was first addressed by Wunch et al. [2011] for ACOS b2.8 and b2.9, who demonstrated the effectiveness of an empirical correction procedure in comparisons to ground truth provided by measurements of the Total Carbon Column Observing Network (TCCON). For ACOS b2.9 we therefore follow the procedure outlined in Equation 4 of Wunch et al. [2011], which leads to a decrease in the absolute values of XCO$_2$ concentrations by 1-2 ppm in the Amazon.

The ACOS team analyzed errors in ACOS b2.10 retrievals and found that some of the correlated biases of ACOS b2.9 remained, while others were reduced. The following equation is therefore recommended to correct ACOS b2.10 land gain H soundings:

$$XCO'_{2} = XCO_{2} + 0.19 \times (\Delta P_{s} + 1.0 \text{ hPa}) + 7.0 \times (albedo_{strong} - 2.0) + 1.2.$$ 

The bias correction leads to an overall increase in XCO$_2$ relative to uncorrected data, with a slight seasonal dependence.

RemoTeC XCO$_2$ retrievals are bias corrected by a posteriori investigating correlations with various instrumental, observational as well as geophysical parameters. To this end, RemoTeC data coinciding with measurements of the Total Carbon Column Observing Network (TCCON) is collected. Differences between TCCON and RemoTeC XCO$_2$ concentrations are found uncorrelated among most of the tested parameters such as
surface reflectivity, solar elevation, concentration of the interfering absorber H₂O, and the recorded signal level in the O₂ A-band. Non-vanishing correlations persist with retrieved scattering properties of the atmosphere which RemoTeC parameterizes through three parameters describing the amount, the height, and the size distribution of particles in the atmosphere [Butz et al., 2009]. The bias correction uses these three parameters to minimize the difference between TCCON and RemoTeC XCO₂. Bias correction of RemoTeC has larger impact on absolute values of XCO₂ compared to correction of ACOS, with an overall increase of 2-3 ppm.

After annual means and secular trend are removed, we find good agreement of seasonal XCO₂ in Amazonia (Fig. S2) for all months except January and February, with peak values in the dry season (~ July) and minimum values in the wet season (~ January), indicating that seasonality variability is robust to the choice of retrieval product. Seasonal variability is robust to the bias correction procedure, providing additional confidence in satellite retrievals in Amazonia. Recall that sampling frequency and density varies between products (Fig. S1); this is in large part due to the cloud screening procedure, and may explain the large discrepancy during wet months. Although not shown, the standard error about the monthly signal is similar across all products and mostly independent of bias correction procedure. On average, the monthly error of uncorrected (corrected) data is 0.27 (0.26) ppm month⁻¹ in ACOS b2.9, 0.24 (0.24) ppm month⁻¹ in ACOS b2.10, and 0.25 ppm month⁻¹ in NIES. The exception is RemoTeC, which has higher variability in the uncorrected product (0.42 ppm month⁻¹) and reduced variability in the corrected product (0.32 ppm month⁻¹).
To ensure these results are robust for similar soundings, we compare seasonal variations using matching soundings only (Fig. S2 c & d). Although most soundings are lost during wet months, we find good agreement across retrievals and with Fig. S2 a & b.

Next we test sensitivity to quality control techniques. Since this cannot be done across retrieval products due to other differences, we compare ACOS b2.9 using quality control outlined above and that of Wunch et al. [2011], which is slightly stricter. For example, relative to the quality control defined in the User’s guide, Wunch et al. [2011] correction reduced samples globally by ~35% and in the Amazon by 15%, primarily due to lower tolerance for surface pressure errors. Applying this correction changes monthly variations and regional and sub-regional scale by up 1-2 ppm in some months (e.g., Mar 2010 in the dry region), but overall seasonality and secular trend are unchanged (Fig. S2 e & f).
Fig. S2. (Top Row) Comparison of XCO$_2$ retrievals from ACOS b2.9 (black), ACOS b2.10 (green), RemoTeC (cyan), and NIES (magenta), with and without bias correction (solid and dashed, respectively), for region 1 (left column) and region 2 (right column).

Secular trend is removed as in Fig. 1 of main text. Annual means are removed as
follows: (uncorrected) 387.11 ppm from ACOS b2.9, 386.83 from ACOS b2.10, 385.88 from RemoTeC, 387.31 from NIES; (corrected) 386.01 from ACOS b2.9, 387.19 from ACOS b2.10, and 387.94 from RemoTeC. (middle row) Similar to top row except using matching soundings. Annual means are removed from each product as follows: 386.28 ppm from ACOS b2.9, 386.86 from ACOS b2.10, 387.94 from RemoTeC. (bottom row) Same as Fig. 1 of main text, except open symbols are ACOS b2.9 screened using quality control (QC) described in Table B1 of Wunch et al. [2011].

B. Sampling Bias

Satellite measurements of total column carbon over the Amazon may introduce sampling biases of 1 ppm or larger when averaged over large spatial and temporal scales due to systematic sampling of clear sky conditions [Corbin et al., 2008]. To test for spatial and temporal sampling biases associated with GOSAT, we sample CarbonTracker 2011 [Peters et al., 2007] concentration data according to ACOS b2.9 (CT XCO₂), and compare to the mean of the complete dataset (CT). We find systematic differences between CT and CT XCO₂ between 1 and 2 ppm in Region 1 and approaching 1 ppm in Region 2 (Fig. S3), consistent with Corbin et al. [2008]. The largest biases occur in the wet season when the total number of samples is reduced by a factor of 10-100.
**Fig. S3.** Estimate of possible sampling biases associated with GOSAT ACOS b2.9.

Regionally averaged CarbonTracker 2011 XCO\textsubscript{2} is plotted in black and CT XCO\textsubscript{2} sampled at ACOS b2.9 soundings in blue. CT data is taken from [http://carbontracker.noaa.gov](http://carbontracker.noaa.gov). The right y-axis is a histogram showing the total number of ACOS b2.9 samples per month.
We constrain GPP against solar induced midday retrievals of SIF from GOSAT using the slope of linear fit between SIF and ecosystem model estimates of GPP in the annual average. The empirical linear relationship between GPP and SIF is mechanistically supported by the radiative transfer model, SCOPE [Van der Tol et al., 2009], where SIF and GPP are both proportional to absorbed radiation. Details of GPP calculations are described below.

**A. Retrievals of Chlorophyll Fluorescence**

SIF is retrieved according to Frankenberg et al. [2011a, b], who use a least squares fitting technique that exploits strong Fraunhofer lines outside the $O_2$ A-band. A critical step in the retrieval for this study is the correction for zero-level offset in acquired GOSAT $O_2$ A-band spectra, which minimizes SIF bias at low solar zenith angles such as over the Amazon. The total number of SIF retrievals in one year per 2.5°x2° grid box in the Amazon is shown in Fig. S4. For comparison of midday SIF retrievals with monthly GPP, SIF in converted to daily averages using the technique described in Frankenberg et al. [2011b], which accounts for overpass time, length of day, and variability of the solar zenith angle.
**Fig. S4.** Number of SIF retrievals over Amazon from ACOS-GOSAT from July 2009 through December 2010, aggregated over 2.5°x2° grid boxes.

**B. GPP and SIF are proportional to absorbed radiation**

GPP can be represented by a light-use efficiency (LUE) parameterization as the following equation:

\[ GPP = PAR \cdot fPAR \cdot \varepsilon_p \]  \hfill (1)

where \( PAR \) is the incident flux of light, \( fPAR \) is the fractional absorption of the incoming light, \( \varepsilon_p \) is the efficiency with which light is used in photosynthesis. Typically about 1%
of the quanta absorbed by chlorophyll are re-emitted at longer wavelengths as fluorescence. As a first approximation the flux of SIF detected by the satellite sensor can be expressed by an equation that is analogous to the expression for GPP,

\[ F_s = \text{PAR} \cdot f\text{PAR} \cdot \varepsilon_f \] (2)

where \( \varepsilon_f \) is analogous to the light-use efficiency in Eqn. 1 but takes into account both the yield of fluorescence at the leaf level and fraction of it that is captured by the satellite.

These equations can be combined and rearranged to give,

\[ \text{GPP} = F_s \cdot \frac{\varepsilon_p}{\varepsilon_f} \] (3)

showing that GPP and SIF will have linear relationship when variation in \( \varepsilon_p \) and \( \varepsilon_f \) are parallel tending to keep the ratio \( \varepsilon_p \cdot \varepsilon_f \) constant.

C. Testing for Sampling Biases in Chlorophyll Fluorescence

SIF retrievals are available as midday clear sky “snapshots” and isolated to a subset of days within a month due to screening for high optical depth and 3-day sampling period.

Since we regress SIF retrievals against monthly average GPP from models, it is necessary to test whether (1) midday SIF is representative of the diurnal cycle, (2) 3-day sampling produces biases in the monthly average. Since SIB3 is available at 10-minute resolution and GPP is well correlated with SIF, we use midday SIB3 GPP as a proxy to test for sampling biases related to (1) and (2) above. Although daily average GPP is always smaller than the corresponding midday value due to overnight averaging, daily average and midday GPP are well correlated at global scales \( R^2 = 0.95 \) for all vegetated land points, Fig. S5a). Scaling midday GPP to the daily average using the technique described
in Frankenberg et al. [2011b] produces a low bias relative to the “true” daily average from SIB3 (Fig. S5b); however, reduced scatter and higher correlation ($R^2 = 0.97$ for all points) indicates that sampling SIF at midday and scaling by the cosine of the solar zenith angle produces reasonable (albeit low) estimate of the daily average. Similarly, this technique produces reasonable estimates of the monthly average ($R^2 = 0.97$, Fig. S5c), although GPP may be low by 10-20%.
Fig. S5. Scatter-plot of 4° x 4° grid cell averages of SIB3 based GPP for (A) daily average GPP ($GPP_{Daily}$) versus midday GPP ($GPP_{Inst}$), (B) $GPP_{Daily}$ versus $GPP_{Inst}$ scaled to the daily average ($GPP_{Inst}$), and (C) monthly average GPP ($GPP_{Monthly}$) versus $GPP_{Inst}$. Black dots are grid boxes over vegetated areas. Red dots are Amazon samples.
D. Calibration GPP Models

SIF is calibrated against three ecosystem models: MPI-BGC, CASA-GFED, and SIB3. MPI-BGC is derived from direct eddy-covariance flux tower measurements and includes a correction for energy imbalance. Flux tower density is generally lower in the Amazon and likely not as representative as other regions, but these and other uncertainties are taken into account, resulting in a product with much smaller spread in the tropics than process-oriented biosphere models. CASA-GFED [van der Werf et al., 2010] is a light use efficiency (LUE) ecosystem model that estimates net primary production (NPP) using relationships between LUE and the fraction of Photosynthetically Active Radiation (fPAR), which is calculated from the Global Inventory Modeling and Mapping Studies (GIMMS) Normalized Difference Vegetation Index (NDVI) [Los et al., 2000]. GPP is approximated as 2 x NPP [Prentice et al., 2001]. SIB3 is an enzyme kinetics model that parameterizes photosynthetic carbon assimilation based on enzyme kinetics developed by Farquhar et al. [1980] and is linked to stomatal conductance to balance GPP against water loss through leaf stomata [Collatz et al., 1991, 1992]. Leaf area index and fPAR, which are used to scale leaf-level photosynthesis up to the ecosystem, are prescribed from MODerate-resolution Imaging Spectroradiometer (MODIS) [Zhao et al., 2005]. Seasonal plots of GPP in regions 1 and 2 for each model are shown in Fig. S7.

Fig. S6 shows the scatter of fit of SIF with GPP from each ecosystem model. The regression is approximately linear in all cases, with SIB3 and CASA-GFED3 becoming slightly non-linear at higher values of SIF. The slope of fit is highest with respect to MPI-BGC (GPP increases by 15.84 gC m$^{-2}$ d$^{-1}$ for every 1.0 W m$^{-2}$ um$^{-1}$ sr$^{-1}$ increase in
SIF), but only slightly weaker for SIB3 and CASA-GFED3 (14.23 and 15.22, respectively). MPI-BGC has weaker scatter than SIB3 and CASA-GFED3, reflected in the higher correlation and smaller error.

**Fig. S6.** Scatter-plot of 4° x 4° grid cell averaged monthly GPP against daily averaged GPP scaled by the cosine of the solar zenith angle for (A) MPI-BGC, (B) SIB3, and (C) CASA-GFED3. Black dashed line is linear fit to all points (blue dots), black solid lines are 1-σ error, and red dotted line is 2nd order fit. Red dots indicate points in Amazonia.
E. Analysis of GPP

Seasonal plots of model GPP and SIF scaled by model GPP are shown for eco-region in Fig. S7. In both regions and in models and SIF, GPP decreases during the dry season, indicating sensitivity of photosynthetic uptake to increased water stress during seasonal drought [Lee et al., in review]. We note the dry season GPP decrease in region 1 is much stronger in SIF than in models. There is also strong reduction in model variance and coherence of seasonality among estimates of GPP. We note that the discrepancy between annual mean observed and model GPP is related to the use of global data in the calculation of the linear slope between SIF and GPP. Amazon GPP is on average larger than the global average (see Fig. S6), which leads to a low bias in our Amazon estimates since global data is used to compute scaling factors.
Fig. S7. Seasonal GPP aggregated over (a) region 1 and (b) region 2 (regions described in Fig. 1 of main text). Black lines represent model GPP from MPI (solid), SIB3 (dashed), and CASA-GFED3 (dotted). Green lines represent SIF scaled to GPP using slope of linear fit with MPI, SIB3, and CASA-GFED3.
Correlation and slope of monthly mean grid scale XCO₂ and observed GPP for Amazon sub-regions are shown in Tab. S1. This table includes statistics for all retrieval products, with and without bias correction.

<table>
<thead>
<tr>
<th>Retrieval</th>
<th>Raw or BC?</th>
<th>r</th>
<th>slope (ppm / gC m⁻² d⁻¹)</th>
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<td>Raw</td>
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<td>-0.30 (-0.10)</td>
</tr>
<tr>
<td>ACOS b2.10</td>
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<td>-0.19 (-0.16)</td>
</tr>
<tr>
<td>RemoTeC</td>
<td>Raw</td>
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<td>-0.14 (-0.13)</td>
</tr>
<tr>
<td>NIES</td>
<td>Raw</td>
<td>+0.35 (+0.00)</td>
<td>+0.45 (+0.00)</td>
</tr>
<tr>
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<tr>
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</tr>
<tr>
<td>NIES</td>
<td>BC</td>
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Tab. S1. Estimates of correlation (r) and slope of regression (slope) between 2.5° x 2° grid scale values of monthly mean observed GPP (as estimated from SIF) and detrended XCO₂ for raw (Raw) and bias corrected (BC) versions of retrieval products. The first number in columns 3 and 4 represent values for region 1. The second number (in parenthesis) represents region 2.
The seasonal pattern of carbon monoxide variability from L3 monthly mean MOPITT (Version 93.1.3, obtained from http://eosweb.larc.nasa.gov/PRODOCS/mopitt/table_mopitt.html on March 7, 2012) aggregated over Amazonia is shown in Fig. S8. Data from August and September 2009 is missing.

Fig. S8. Seasonal time series of column integrated carbon monoxide from MOPITT, averaged across the Amazon.
References for Supplementary Online Material


11. Lee et al. [in review]


