

1 Prior biosphere model impact on global terrestrial CO₂ fluxes estimated 2 from OCO-2 retrievals

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16 **Abstract.** This study assesses the impact of different state-of-the-science global biospheric CO₂ flux models, when applied as prior
17 information, on inverse model “top-down” estimates of terrestrial CO₂ fluxes obtained when assimilating Orbiting Carbon
18 Observatory 2 (OCO-2) observations. This is done with a series of Observing System Simulation Experiments (OSSEs) using
19 synthetic CO₂ column-average dry air mole fraction (XCO₂) retrievals sampled at the OCO-2 satellite spatio-temporal frequency.
20 The OSSEs used a four-dimensional variational (4D-Var) assimilation system with the GEOS-Chem global chemical transport
21 model (CTM) to estimate CO₂ net ecosystem exchange (NEE) fluxes using synthetic OCO-2 observations. The impact of biosphere
22 models in inverse model estimates of NEE is quantified by conducting OSSEs using the NASA-CASA, CASA-GFED, SiB-4 and
23 LPJ models as prior estimates and using NEE from the multi-model ensemble mean of the Multiscale Synthesis and Terrestrial
24 Model Intercomparison Project as the “truth”. Results show that the assimilation of simulated XCO₂ retrievals at OCO-2 observing
25 modes over land results in posterior NEE estimates which generally reproduce “true” NEE globally and over terrestrial TransCom-
26 3 regions that are well-sampled. However, we find larger spread among posterior NEE estimates, when using different prior NEE
27 fluxes, in regions and seasons that have limited OCO-2 observational coverage and a large range in “bottom-up” NEE fluxes.
28 Seasonally-averaged posterior NEE estimates had standard deviations (SD) of ~10% to ~50% of the multi-model-mean NEE for
29 different TransCom-3 land regions with significant NEE fluxes (regions/seasons with a NEE flux ≥ 0.5 PgC yr⁻¹). On a global
30 average, the seasonally-averaged residual impact of the prior model NEE assumption on posterior NEE spread is ~10-20% of the
31 posterior NEE mean. Additional OCO-2 OSSE simulations demonstrate that posterior NEE estimates are also sensitive to the
32 assumed prior NEE flux uncertainty statistics, with spread in posterior NEE estimates similar to those when using variable prior
33 model NEE fluxes. In fact, the sensitivity of posterior NEE estimates to prior error statistics was larger compared to prior flux
34 values in some regions/times in the Tropics and Southern Hemisphere where sufficient OCO-2 data was available and large
35 differences between the prior and “truth” were evident. Overall, even with the availability of spatio-temporally dense OCO-2 data,
36 noticeable residual differences (up to ~20-30% globally and 50% regionally) in posterior NEE flux estimates remain that were
37 caused by the choice of prior model flux values and the specification of prior flux uncertainties.

1 **1 Introduction**

2 Carbon dioxide (CO₂) is the most important greenhouse gas (GHG) contributing to climate change on a global scale (IPCC, 2014).
3 The anthropogenic emission of CO₂, primarily from fossil fuel usage, has led to average global CO₂ mixing ratios reaching
4 historically high levels of > 400 parts per million (ppm) (Seinfeld and Pandis, 2016). In addition to fossil fuel emissions, the
5 processes involved in the exchange of carbon between the atmosphere and terrestrial biosphere are a major factor controlling
6 atmospheric concentrations of CO₂ (e.g., Schimel et al., 2001) with an estimated global biosphere sink of ~3.0 PgC yr⁻¹ (Le Quéré
7 et al., 2018). However, current estimates of regional-scale atmosphere-terrestrial biosphere CO₂ exchange have large uncertainties
8 (Schimel et al., 2015). “Bottom-up” techniques typically simulate the atmosphere-terrestrial biosphere exchange based on our
9 understanding of these complex exchange processes and by constraining these estimates with remote-sensing inputs and limited
10 measurements available for evaluation. Previous studies inter-comparing several of the most commonly used biospheric flux
11 models (Heimann et al., 1998, Huntzinger et al., 2012; Sitch et al., 2015; Ott et al., 2015; Ito et al., 2016) and multi-model ensemble
12 integration projects (Schwalm et al., 2015) reveal a large spread among global/regional “bottom-up” terrestrial biospheric flux
13 estimates and the sub-components such as ecosystem primary production and respiration (Huntzinger et al., 2012).

14 An alternate approach to estimate biospheric CO₂ fluxes is through “top-down” estimation techniques using inverse
15 models with highly accurate in situ data (e.g., Baker et al., 2006b) or dense and globally distributed satellite data (e.g., Chevallier
16 et al., 2005). The Orbiting Carbon Observatory 2 (OCO-2) satellite, launched in 2014, is the space-borne sensor with the finest
17 resolution and highest sensitivity of CO₂ in the atmospheric boundary layer to date (Crisp et al., 2017; Eldering et al., 2017a).
18 Studies applying OCO-2 retrievals revealed the ability to investigate novel aspects of the carbon cycle (e.g., Eldering et al., 2017b;
19 Liu et al., 2017), however, the “top-down” estimates of surface CO₂ fluxes from numerous inverse modeling systems, using
20 identical OCO-2 observations, show differences among optimized/posterior regional CO₂ fluxes (Crowell et al., 2019). Previous
21 studies investigating CO₂ flux inversions (e.g., Peylin et al., 2013; Chevallier et al., 2014; Houweling et al., 2015) suggest that this
22 spread among optimized CO₂ flux estimates could be due to numerous factors, such as the accuracy and precision of observation
23 data (Rödenbeck et al., 2006), imperfect observation coverage (Liu et al., 2014; Byrne et al., 2017), data density (Law et al., 2003;
24 Rödenbeck et al., 2003) and poorly characterized measurement error covariance (Law et al., 2003; Takagi et al., 2014). Variations
25 in inverse estimation setups between modeling groups, such as model transport (Chevallier et al., 2010; Houweling et al., 2010;
26 Basu et al., 2018) and inversion methods (Chevallier et al., 2014; Houweling et al., 2015), could also lead to inter-model spread in
27 posterior estimates.

28 In addition to the variables listed above, the assumed prior fluxes and the associated prior error covariance can also impact
29 “top-down” global/regional CO₂ flux estimates (e.g., Gurney et al., 2003). Gurney et al. (2003) assessed the sensitivity of CO₂ flux
30 inversions to the specification of prior flux uncertainty and found that the posterior estimates were sensitive to the prior fluxes over
31 regions with limited in situ observations. In addition, Wang et al. (2018) found that optimal CO₂ flux allocation over land versus
32 ocean, using satellite and/or in situ data assimilations, is sensitive to the specification of prior flux uncertainty. Furthermore,
33 Chevalier et al. (2005) and Baker et al. (2006a; 2010) highlighted the importance of accurate assumptions of prior flux uncertainty
34 by conducting four-dimensional variational (4D-Var) assimilations of satellite column retrievals of CO₂. However, to date, there
35 are no controlled experimental studies to isolate and quantitatively assess the impact of assumed prior fluxes and prior uncertainty
36 to inverse estimates of biospheric CO₂ fluxes using satellite observations.

37 Therefore, during this study we conduct a series of controlled experiments to quantitatively assess the impact of assumed
38 prior fluxes and prior uncertainty on global and regional CO₂ inverse model flux estimates when assimilating OCO-2 data. In order
39 to achieve this, a series of Observing System Simulation Experiments (OSSEs) are conducted using synthetic OCO-2 observations
40 in the GEOS-Chem 4D-Var assimilation system, with four different prior “bottom-up” NEE CO₂ flux estimates. Section 2 of this

1 study describes the methods applied during this work including individual models and model input, synthetic OCO-2 data and the
2 inversion technique applied in the OSSEs. Section 3 presents the forward and inverse model results of simulated atmospheric CO₂
3 concentrations and inferred posterior flux estimates. Finally, our concluding remarks and discussion are presented in Section 4.

4 **2 Methods**

5 To quantify the impact of prior model NEE predictions on posterior estimates of biospheric CO₂ fluxes, a series of CO₂ forward
6 and inverse model simulations were conducted with four different state-of-the-science biosphere models. OSSE simulations were
7 designed to isolate the differences in posterior NEE estimates caused by the selection of prior model biospheric CO₂ fluxes and
8 uncertainties when assimilating OCO-2 observations. The OSSE framework, input variables, inversion technique and analysis
9 method are presented below.

10 **2.1 Prior NEE fluxes**

11 NEE is the net difference of gross primary production (GPP) and total ecosystem respiration (R_e), which itself is the sum of
12 autotrophic respiration (R_a) and heterotrophic respiration (R_h). NEE, estimated by terrestrial biospheric CO₂ flux models, is
13 commonly applied in CTMs to simulate atmosphere-terrestrial biosphere carbon exchange. Many biosphere carbon models
14 estimate GPP and R_e , however, some models simulate net primary productivity (NPP), which is defined as the difference between
15 GPP and R_a . In this study, we apply year-specific NEE fluxes calculated from four state-of-the-science biosphere models: 1) NASA
16 Carnegie Ames Stanford Approach (NASA-CASA), 2) CASA-Global Fire Emissions Database (CASA-GFED), 3) Simple-
17 Biosphere model version 4 (SiB-4) and 4) Lund-Potsdam-Jena (LPJ). It should be noted that the prior biosphere models used in
18 this study include only NEE and a single dataset for wild fire and fuel wood burning CO₂ emissions was added separately (see
19 Sect. 2.3). The models applied during this study represent a range of diagnostic approaches, from models predicting biospheric
20 CO₂ fluxes using remotely-sensed data (e.g., Fraction of Absorbed Photosynthetically Active Radiation, Leaf Area Index,
21 Normalized Difference Vegetation Index) to fully prognostic models unconstrained by observations. In addition, we selected both
22 balanced/neutral (SiB-4) and non-balanced (NASA-CASA, CASA-GFED, LPJ) biospheric fluxes in our OSSEs in order to
23 represent the range of prior models currently being used in CO₂ inversion modeling studies.

24 CASA is an ecosystem model predicting NPP based on light use efficiency and R_h based on soils/plant production
25 information (Potter et al., 1993; 2012b). The NASA-CASA model is a version of the original CASA model (Potter et al., 1993)
26 currently being developed at NASA Ames Research Center (Potter et al., 2003; 2007; 2009; 2012a; 2012b). NASA-CASA
27 specifically utilizes data on global vegetation cover (Enhanced Vegetation Index, Surface Solar Irradiance Data) and land
28 disturbances retrieved from the NASA Moderate Resolution Imaging Spectroradiometer (MODIS) satellite (Potter et al., 2012b).
29 In addition to R_h , NASA-CASA includes redistributed crop harvest CO₂ emissions to the atmosphere (Potter et al., 2012b). The
30 CASA-GFED model is a different version of the original CASA model and is described in Randerson et al. (1996) with subsequent
31 versions being described in recent literature (van der Werf et al., 2004; 2006; 2010). NASA-CASA and CASA-GFED differ in the
32 use of input parameters and some of the parameterizations (see Ott et al. (2015) for further description).

33 The SiB-4 model was developed at Colorado State University (Sellers et al., 1986; Denning et al., 1996) with details of
34 the newest versions described in Haynes et al. (2013). This model is a mechanistic, prognostic land surface model that integrates
35 heterogeneous land cover, environmentally responsive prognostic phenology, dynamic carbon allocation and cascading carbon
36 pools from live biomass to surface litter and soil organic matter (Haynes et al., 2013; Baker et al., 2013; Lokupitiya et al., 2009;
37 Schaefer et al., 2008; Sellers et al., 1996). By combining biogeochemical, biophysical and phenological processes, SiB-4 predicts
38 vegetation and soil moisture states, land surface energy and water budgets and the terrestrial carbon cycle. Rather than relying on

1 satellite input data, SiB-4 fully simulates the terrestrial carbon cycle by using the carbon fluxes to determine the above and below-
2 ground biomass, which in turn feed back to impact carbon assimilation and respiration. Similar to NASA-CASA, the SiB4 model
3 redistributes crop harvest CO₂ emission to the atmosphere. Note that we use a balanced (neutral) biospheric NEE flux for the SiB-
4 4 model.

5 The LPJ model is a process-based dynamic global vegetation model (Sitch et al., 2003; Polter et al., 2014). The LPJ-wsl
6 dynamic global vegetation model (Sitch et al., 2003) was used to simulate NEE using meteorological data from the Climate
7 Research Unit (Harris et al., 2013). LPJ is fully prognostic, meaning that the establishment, growth and mortality of vegetation are
8 represented by first-order physiological principles. The model includes nine plant functional types distinguished by their
9 phenology, photosynthetic pathway and physiognomy. Phenology status is determined daily and photosynthesis is estimated using
10 a modified Farquhar scheme (Haxeltine and Prentice, 1996). NPP is calculated from photosynthesis after accounting for R_a and
11 reproductive allocation. The LPJ-wsl model has been evaluated in several benchmarking activities for stocks and fluxes (Peng et
12 al., 2015; Sitch et al., 2015).

13 In order to provide a “true” NEE flux for the OSSEs conducted in this study (Sect. 2.4), we use the multi-model ensemble
14 NEE mean from the Multiscale Synthesis and Terrestrial Model Intercomparison Project (MsTMIP) (Huntzinger et al., 2013; 2018;
15 Fisher et al., 2016a; 2016b). The MsTMIP NEE fluxes are from a weighted ensemble mean of 15 biosphere models (Schwalm et
16 al., 2015) for the year 2010. Here we apply the MsTMIP data for year 2010 as the “truth” with year-specific prior model predictions
17 for 2015. This procedure is justified in our case as within an OSSE framework there needs to be a difference between “true” and
18 prior fluxes, as long as the “true” values are realistic in nature. The MsTMIP ensemble NEE mean represents a summary over all
19 15 models which smooths out errors particular to any given model. This “true” NEE flux is used to produce the synthetic OCO-2
20 observations applied in this study (described further in Sect. 2.4.3).

21 The “true” and four prior model NEE fluxes were regridded from their native horizontal resolutions to the grid resolution
22 of the inverse model simulations (4.0° latitude × 5.0° longitude). The MsTMIP NEE fluxes are provided as 3-hourly averages and
23 the four year-specific prior models were provided as monthly-mean GPP or NPP and R_e or R_h. Therefore, we imposed diurnal
24 (hourly) and daily variability to these four prior models following the approach in CarbonTracker CT2016
25 (<http://carbontracker.noaa.gov>), which is based on Olsen and Randerson (2004). This hourly/daily NEE variability for each prior
26 model was calculated using the downward solar radiation flux and 2-meter air temperature data from the GEOS-FP (Goddard Earth
27 Observing System Model, Version 5 "Forward Processing") meteorological product and monthly-averaged GPP and R_h from the
28 respective model. We allow the “true” and prior models to have different diurnal variability in order to represent a realistic scenario,
29 as prior models will differ some from the actual diurnal variability of NEE in nature. In general, the diurnal variability of NEE is
30 similar between the “true” and individual prior models. An example is shown in Fig. S1 where it can be seen that the diurnal NEE
31 from the “true” and prior models for July 2015 at the Park Falls flux tower site (45.95°N, 90.27°W) have near identical temporal
32 diurnal patterns and only differ in NEE magnitude. Table 1 shows the global annual NEE flux estimates for the four prior models
33 and the “truth”. From this table it can be seen that the MsTMIP product shows a strong annual global sink of -4.31 PgC yr⁻¹. NASA-
34 CASA and CASA-GFED predict a global sink of ~2 PgC yr⁻¹ and differ by ~0.6 PgC yr⁻¹. SiB-4 NEE predicts a source of ~1 PgC
35 yr⁻¹ and the LPJ model predicts a strong sink of ~5.5 PgC yr⁻¹. Section 3.1 further describes the spatio-temporal differences of the
36 NEE fluxes between these four prior models and the “truth”.

37 **2.2 GEOS-Chem model**

38 The GEOS-Chem chemical transport model (CTM) (<http://geos-chem.org>; Bey et al., 2001) used in this study has the capability to
39 run forward CO₂ simulations (Suntharalingam et al., 2004; Nassar et al., 2010) and corresponding adjoint model calculations

1 (Henze et al., 2007; Liu et al., 2014). In this study, we use the GEOS-Chem adjoint version 35, which is compatible with version
2 8-02 of the GEOS-Chem forward model. Liu et al. (2014) tested the accuracy of the GEOS-Chem CO₂ adjoint system, which has
3 been used for several CO₂ inverse modeling studies (e.g., Liu et al., 2017; Bowman et al., 2017; Deng et al., 2014). The model is
4 driven with assimilated meteorological fields from the GEOS-FP model of the NASA Global Modeling Assimilation Office
5 (GMAO). The GEOS-FP meteorology fields have a native horizontal resolution of 0.25° × 0.3125° and 72 native hybrid sigma-
6 pressure vertical levels from the Earth’s surface to 0.01 hPa. We conduct simulations with a coarser spatial resolution (4.0° × 5.0°)
7 with 47 reduced vertical levels to attain reasonable computational efficiency.

8 **2.3 Non-NEE CO₂ fluxes**

9 To simulate concentrations of atmospheric CO₂, we used several land and ocean CO₂ flux inventories in addition to the NEE
10 estimates from the prior biosphere models (global annual budgets listed in Table 1). This study used the year-specific fossil fuel
11 and cement production inventory from the Open-source Data Inventory for Anthropogenic CO₂ (ODIAC-2016) developed by Oda
12 et al. (2018). Following the approach of Nassar et al. (2013), the monthly ODIAC-2016 inventory is converted from the native
13 temporal variability into diurnal (hourly) and weekday/weekend variability (courtesy: Sourish Basu and the OCO-2 Science Team).
14 Wild fire emissions and fuel wood burning emissions were taken from the 3-hourly Global Fire Emissions Database (GFED3)
15 database. Shipping emissions are from the International Comprehensive Ocean-Atmosphere Data Set (ICODS) (Corbett and
16 Koehler, 2003; 2004) and aviation emissions are from the Aviation Emissions Inventory Code (AEIC) inventory (Olsen et al.,
17 2013). We used 3D chemical production of CO₂ from the oxidation of carbon monoxide, methane and non-methane volatile organic
18 compounds (Nassar et al., 2010). The shipping, aviation and 3D chemical source are climatological and are taken from the Bowman
19 (2017) dataset. To simulate oceanic CO₂ fluxes, we apply the year-specific 3-hourly posterior estimates from the CarbonTracker
20 2016 (CT2016) model constrained with in situ data (Peters et al., 2007; <http://carbontracker.noaa.gov>). All emission inventories,
21 besides NEE fluxes, are kept constant between the different inverse model simulations.

22 **2.4 Observing System Simulation Experiments (OSSEs)**

23 **2.4.1 OSSE framework**

24 This study conducted several OSSEs to assess the impact of prior biospheric CO₂ models and associated prior uncertainty
25 specifications on posterior estimates of NEE when assimilating OCO-2 data. To assess the impact of prior fluxes, we conduct four
26 baseline OSSEs (using the four prior biosphere models) assimilating synthetic land nadir (LN) and land glint (LG) observations
27 together, plus an additional four OSSEs using just ocean glint (OG) observations. These OSSE simulations were designed in such
28 a way that the differences in posterior NEE estimates are due solely to the choice of prior biospheric flux (e.g., identical initial
29 atmospheric CO₂ conditions, non-NEE fluxes, OCO-2 sampling frequency, observational data uncertainty, etc.). Furthermore, to
30 assess the impact of prior uncertainty specifications, we conduct two additional OSSEs (in addition to our baseline prior uncertainty
31 assumption described in Sect. 2.4.5) with synthetic LN and LG observations using prior error set uniformly to 10% and 100% of
32 a particular prior NEE flux (CASA-GFED). Table 2 shows the summary of OSSEs conducted for this study. During all OSSE
33 simulations NEE and oceanic CO₂ fluxes are optimized, with all other sources kept constant, in order to be consistent with the
34 methods commonly used by inverse modeling systems focused on estimating NEE. We optimize oceanic fluxes together with NEE,
35 although the same ocean fluxes were used for the “truth” and the prior in all OSSE simulations (Sect. 2.3) for simplicity and
36 because the terrestrial NEE fluxes are the focus of this work. It is noteworthy that the assimilation of land or ocean data in fact do
37 not produce substantial deviations from the “truth” over the TransCom-3 oceanic regions (Fig. S2). For all OSSE simulations, an
38 assimilation window of 18 months covering the period from August 1, 2014 to January 31, 2016 was applied. NEE/oceanic fluxes

1 are optimized for every month of the assimilation window at each surface grid box in the GEOS-Chem model. The analysis of
2 prior and posterior NEE fluxes is for all months in 2015, treating the other months as spin-up and spin-down periods.

3 **2.4.2 Initial CO₂ concentrations**

4 We use identical initial atmospheric concentrations of CO₂ on August 1, 2014 for: 1) the GEOS-Chem forward model simulations
5 generating synthetic XCO₂ using the “true” NEE fluxes (Sect. 2.4.3) and 2) for all the OSSEs using variable prior biosphere model
6 predictions. The initial CO₂ concentrations were generated by running the GEOS-Chem forward model for two years using the
7 “true” MsTMIP NEE and other non-NEE CO₂ sources. The restart file used for this two year forward model run was taken from
8 an earlier GEOS-Chem model simulation constrained with in situ observations (personal communication from Ray Nassar) in order
9 to represent a realistic initial condition.

10 **2.4.3 Synthetic OCO-2 retrievals**

11 In this study, we used synthetic satellite data that is directly representative of version 8 of the OCO-2 product. The OCO-2 satellite
12 sensor is in sun-synchronous polar orbit with a repeat cycle of 16 days and a local over-pass time in the early afternoon (Crisp et
13 al., 2017). OCO-2 has three different viewing modes: soundings over land from LN and LG and over oceans from OG. The
14 algorithm of O’Dell et al. (2012) is used to retrieve column-average dry air mole fraction of CO₂ (XCO₂) and other retrieval
15 variables. The retrieval of OCO-2 XCO₂ is expressed as Eq. (1) using a prior CO₂ vertical profile (\mathbf{c}_a) and prior CO₂ column
16 (XCO_{2(a)}) value,

$$17 \quad XCO_2 = XCO_{2(a)} + \mathbf{a}^T(\mathbf{c} - \mathbf{c}_a) \quad (1)$$

18 where \mathbf{c} is the true profile of CO₂ concentrations and \mathbf{a} is the column averaging kernel. The individual soundings of OCO-2 are at
19 a fine-resolution (24 spectra per second with < 3 km² spatial resolution per sounding), leading to a very large data volume (Crisp
20 et al., 2017). This level of detail is lost when the measurements are used in global inverse models with much coarser spatial
21 resolution, with numerous individual OCO-2 soundings occur in a single model grid box. In addition, each sounding does not
22 really provide an independent piece of information to the inversion system due to spatial and temporal error correlations. Therefore,
23 we use 10-sec averages of the individual XCO₂ soundings similar to those developed/described in Basu et al. (2018), however,
24 from an updated version with file name: OCO2_b80_10sec_WL04_GOOD_v2.nc. This 10-sec data contains averages of retrievals
25 with a “GOOD” quality flag and Warn Level from 1 to 4. Note that in this study we do not use actual retrieved 10-sec XCO₂ values
26 for our OSSEs, however, synthetic XCO₂ data were generated corresponding to the spatio-temporal sampling frequency of version
27 8 OCO-2 10-sec data. The synthetic 10-sec XCO₂ data is calculated with the CO₂ concentration profile simulated using the GEOS-
28 Chem forward model (using MsTMIP as the NEE flux model). In this manner we produced synthetic XCO₂ data that is
29 representative of the “true” atmosphere corresponding to the “true” NEE fluxes used in this study. We archived these synthetic
30 XCO₂ data and applied them for all OSSEs conducted.

31 **2.4.4 Inverse modeling approach**

32 The transport of atmospheric CO₂ is simulated using GEOS-Chem along with prescribed surface fluxes as input data (see Table
33 1). Subsequently, the GEOS-Chem 4D-Var inverse modeling system assimilates synthetic OCO-2 XCO₂ data to estimate the
34 posterior/optimized monthly-mean NEE and oceanic fluxes at each surface grid box of the model. The GEOS-Chem adjoint system
35 applies the L-BFGS numerical optimization algorithm with a no-bound option (Liu and Nocedal, 1989). Posterior monthly-
36 averaged NEE/oceanic fluxes (\mathbf{x}) are inferred for each surface model grid box by optimizing a vector of scaling factors σ_j for the
37 j^{th} model grid box,

$$x_j = \sigma_j x_{a,j} \quad (2)$$

where \mathbf{x}_a represents the monthly-mean prior NEE/oceanic fluxes. Scaling factors are assumed to be unity at the first iteration (that is, prior NEE flux itself is used). The inversion system, as described below, optimizes the scaling factor applied to the monthly-mean fluxes and the posterior scaling factors are then used to scale prior fluxes to infer posterior CO₂ fluxes.

For each iteration, the inversion system uses the forward model simulated profiles of CO₂ concentrations mapped to OCO-2 retrieval levels ($\mathbf{f}(\mathbf{x})$) in each model grid box in order to compare with the synthetic OCO-2 observations (\mathbf{y}). The observation operator (\mathbf{M}) represents the model simulated XCO₂ corresponding to each synthetic OCO-2 retrieval,

$$\mathbf{M} = \text{XCO}_{2(a)} + \mathbf{a}^T (\mathbf{f}(\mathbf{x}) - \mathbf{c}_a) \quad (3)$$

using $\text{XCO}_{2(a)}$ and \mathbf{c}_a from the retrieval (see Eq. (1)). The optimization approach used in this work defines the 4D-Var cost function (J) as,

$$J(\boldsymbol{\sigma}) = \frac{1}{2} \sum_i (\mathbf{M}_i - \mathbf{y}_i)^T \mathbf{R}_i^{-1} (\mathbf{M}_i - \mathbf{y}_i) + \frac{1}{2} (\boldsymbol{\sigma} - \boldsymbol{\sigma}_a)^T \mathbf{P}^{-1} (\boldsymbol{\sigma} - \boldsymbol{\sigma}_a) \quad (4)$$

where \mathbf{y}_i is the vector of synthetic OCO-2 XCO₂ data across the assimilation window, with ‘ i ’ being the number of XCO₂ data. Furthermore, \mathbf{R} and \mathbf{P} are the observational error covariance matrix and prior error covariance matrix, respectively.

2.4.5 Prior flux uncertainty

For a perfect optimization, the prior error covariance matrix (\mathbf{P}) assumed in the inversion should equal the uncertainty of the prior model used. However, the estimation of prior error statistics is a challenging task due to the lack of flux evaluation data. Previous studies have used a range of techniques to characterize prior error covariance: by developing the full error covariance matrix with assumed error correlations (Basu et al., 2013), based on a fraction of heterotrophic respiration (Basu et al., 2018), conducting Monte Carlo simulations (Liu et al., 2014), using standard deviations and absolute differences between several different prior flux models (Baker et al., 2006a; 2010), using continuous in situ measurements of CO₂ flux compared to model simulations to inform prior errors (Chevallier et al., 2006) and applying globally uniform prior flux uncertainty values to satisfy the posterior χ^2 (normalized cost function) = 1 criteria (Deng et al., 2014). During this study, a 1σ standard deviation (SD) of the four prior biosphere models (see Sect. 3.1 for the description of SD values) is considered to be the measure of uncertainty in the prior knowledge of “bottom-up” model predicted biospheric CO₂ fluxes. The SD of the four prior NEE estimates is applied in the prior error covariance matrix and no spatial or temporal correlations are taken in to account. This assumption is reasonable as optimized fluxes are at coarse spatio-temporal scales (monthly mean fluxes at horizontal resolutions of $> 400 \text{ km}^2$) and is representative of the majority of inverse modeling studies assimilating CO₂ satellite data (e.g., Baker et al., 2010; Liu et al., 2014; Deng et al., 2014). Finally, since the inverse modeling system applied in this work optimizes scaling factors, we use the square of the fractional prior error in the \mathbf{P} matrix, where the fractional error is calculated for each individual prior model as the SD of the four prior models divided by the absolute value of the NEE magnitude. For generating prior error for the oceanic fluxes, we follow the same method we adopted for generating prior errors in NEE. The SD of four different state-of-the-science oceanic CO₂ flux datasets (NASA-CMS CO₂ oceanic flux from Bowman (2017), CarbonTracker 2016 prior ocean data (CT2016; <http://carbontracker.noaa.gov>), Takahashi et al. (2009) and Landschützer et al. (2016; 2017)) was calculated to generate prior error values.

2.4.6 XCO₂ uncertainty

As described in Sect. 2.4.3, the synthetic XCO₂ used in this study is calculated at the spatio-temporal sampling frequency of OCO-2 10-sec average dataset. Although we use synthetic XCO₂, we apply the same observation error statistics generated with the actual OCO-2 XCO₂ 10-sec dataset in order to develop the observational error covariance matrix (\mathbf{R}). The final observation error for the

1 10-sec average data is generated as a quadratic sum of the retrieval error from individual OCO-2 soundings, 10-sec averaging error,
2 and a ‘model representation error’ as described in Basu et al. (2018). Similar to the treatment of prior error statistics, we neglect
3 observation error correlations and assume a diagonal observational error covariance. No random perturbations were added to the
4 synthetic XCO₂ used in this study, as the goal of this work was not to quantify the analytical posterior flux uncertainty but instead
5 was aimed to analyze the spread among posterior NEE estimates. We note that other inverse modeling groups assimilating OCO-
6 2 data also do not add random perturbations to the data and use the same error statistics generated along with the OCO-2 10-sec
7 product that are applied in this study (e.g., Basu et al., 2018; Crowell et al., 2019). During this study the square of the observation
8 error for the 10-sec average data was applied as the diagonal in the **R** matrix. From our initial OSSE tests it was determined that
9 the use of 10-sec error statistics led to posterior χ^2 (normalized cost function) values that were much lower than unity. Therefore,
10 we divided the 10-sec error values uniformly by a factor of 5 to approximately satisfy the $\chi^2 = 1$ criteria for all the OSSEs. This
11 deflation procedure reduced the average 10-sec observational error values for LN+LG (OG) data from ~1.5 (~0.9) ppm to ~0.3
12 (~0.2) ppm. These procedures give more confidence to the observational data and lead to results in this study which can be assumed
13 as the lower limit of the impact of prior model flux and uncertainty statistics in inverse model estimates.

14 **2.4.7 Evaluation of OSSE results**

15 During this study, the posterior NEE values from the OSSEs are compared to the “true” fluxes to assess accuracy and also inter-
16 compared to assess the spread in posterior estimates due to the assumed prior NEE and prior error statistics. The primary statistical
17 parameters used to evaluate the spread in posterior NEE fluxes are the SD (hereafter the term “spread” will be used to represent
18 SD) and range (difference between maximum and minimum in NEE). The SD/spread and range of posterior NEE estimates, when
19 using the different prior models, will provide an understanding of the spatio-temporal residual impact of the prior models in “top
20 down” estimates of global/regional NEE fluxes when assimilating OCO-2 data.

21 In order to evaluate the spatio-temporal variability of prior and posterior regional NEE fluxes, we aggregate individual
22 model grid boxes to the TransCom-3 land regions (TransCom-3 regions illustrated in Fig. 1). To further interpret the OSSE results,
23 we produce additional classifications of three broad hemisphere-scale TransCom-3 land regions: Northern Land (NL), Tropical
24 Land (TL) and Southern Land (SL). TL includes Tropical South America, North Africa and Tropical Asia; SL includes South
25 American Temperate, South Africa and Australia; and NL includes the other five land regions. The evaluation of SD and range of
26 prior model and posterior/optimized NEE fluxes were calculated for the 11 individual TransCom-3 regions, for the three
27 hemisphere-scale TransCom-3 regions and globally. Throughout the manuscript, seasonally-averaged prior and posterior NEE
28 fluxes will be discussed and these seasons are presented with respect to the Northern Hemisphere.

29 **2.4.8 Pseudo data assimilations**

30 In order to test our OSSE framework, we first run four “pseudo” experiments by conducting inverse modeling studies using
31 “pseudo” surface observations. These test OSSE simulations were conducted for five-month assimilation windows for two separate
32 seasons (November 2014 to March 2015 (analysis for winter, DJF) and May 2015 to September 2015 (analysis for summer, JJA))
33 using all four prior model NEE values separately. Simulated hourly concentrations of CO₂ for all surface grid boxes of GEOS-
34 Chem are taken as “pseudo” surface observations. In order to check whether the model framework can converge to the “truth”, a
35 simple controlled experiment was performed assuming a very small observational data uncertainty (0.001%) and with the prior
36 flux uncertainty set equal to the absolute magnitude of the “truth” - prior NEE (divided by the absolute value of the NEE magnitude
37 for that respective prior model). The robustness of the flux inversions conducted in the subsequent sections is validated by the
38 results of these “pseudo” tests. Figure S3 shows the results of the four “pseudo” tests using the four different NEE flux model

1 predictions as the prior information. From this figure it is apparent that, regardless of the prior NEE assumed, posterior NEEs were
2 able to reproduce the “truth” with near perfect accuracy for all TransCom-3 regions, with the range between the posterior NEEs
3 typically approaching ~ 0 PgC yr⁻¹. This test also demonstrates that a “perfect” assimilation (using uniform and dense surface data
4 coverage, highly accurate data and known/loose prior uncertainty) is almost insensitive to the prior assumed. Having tested the
5 robustness of our inversion setup, we feel confident in presenting the output from our OSSE framework, using synthetic OCO-2
6 remote-sensing data, in the following sections.

7 **3. Results and discussion**

8 **3.1 Prior NEE fluxes**

9 Figure 2 shows the seasonally-averaged multi-model-mean and SD of the NEE fluxes from the four prior biosphere models used
10 in the OSSE simulations (individual prior model and “true” seasonally-averaged NEE fluxes are displayed in Fig. S4). This figure
11 shows the main features of NEE that are expected, such as the Northern Hemispheric fall/winter maximum in R_e and summer
12 maximum in GPP due to the seasonality of photosynthesis and respiration. Figure 2 also shows the spread of the four prior model
13 fluxes (used as prior uncertainty), which is typically highest over the Temperate regions of the Northern Hemisphere in the spring
14 and summer and high in the Tropical regions during all seasons (the left panel of Figure 3 shows a spatial map of the corresponding
15 range of the four prior model fluxes). Furthermore, Fig. S5 shows the time-series of monthly-mean prior NEE fluxes, and the
16 corresponding prior error uncertainty (error bars), for the individual prior models. From this figure it can be seen that the 1σ prior
17 uncertainties for the global land are ~ 50 - 70% of the total NEE for the different prior models, with variability among other
18 TransCom-3 land regions.

19 Table 3 displays the statistics of the prior NEE multi-model-mean and SD and range for the 11 individual TransCom-3
20 land regions. The SD values for prior NEE fluxes range from $\sim 20\%$ to frequently $> 100\%$ of the multi-model NEE mean for
21 different regions/seasons with significant NEE fluxes (hereafter this refers to regions/seasons with NEE flux ≥ 0.5 PgC yr⁻¹). When
22 comparing the magnitude of NEE between the four prior models, it can be seen from this table that the range in NEE values are
23 large in some regions (up to 6 PgC yr⁻¹). In general, all regions/seasons tend to have at least an ~ 1 PgC yr⁻¹ range among the four
24 prior models, indicating the large diversity in NEE predicted by current “bottom-up” biosphere models (Table 3). Figure S5 shows
25 the time-series of monthly-mean NEE for individual prior models averaged over the globe, hemispheric-scale land regions (NL,
26 TL, SL) and the 11 individual TransCom-3 land regions. It can be seen from this figure that the majority of the seasonality in the
27 global NEE flux is controlled by the NL regions. Figure S5 also shows that the spread in prior NEE fluxes in general is larger for
28 TL and SL regions compared to the NL, except for the North American Temperate region. Furthermore, when focusing on
29 individual models, differences in NEE seasonality are evident. The impact of these differences among the four prior biospheric
30 CO₂ flux models on simulated XCO₂ and posterior estimates of global/regional NEE fluxes is evaluated in the following sections.

31 **3.2 Simulated XCO₂**

32 Figure 4 shows the number of observations sampled in the OCO-2 LN and LG modes during the different seasons of 2015 summed
33 in each model grid box. Large spatio-temporal variability can be seen in the OCO-2 observation density, with the largest values
34 over regions with minimal cloud coverage (e.g., desert regions of North/South Africa, Middle East, Australia, etc.). The opposite
35 is true for many Tropical regions (e.g., Amazon, central Africa, Tropical Asia, etc.) where cloud occurrence is prominent and the
36 number of OCO-2 observations is lowest. From Fig. 4 it can also be seen that the OCO-2 observation density has noticeable
37 seasonality. For example, during the winter months low numbers of OCO-2 observations are made in the Northern Boreal regions

1 and the largest amounts are observed during the summer. Furthermore, larger numbers of OCO-2 observations are made in the SL
2 during the summer (JJA) compared to other seasons.

3 The seasonally-averaged multi-model-mean GEOS-Chem simulated XCO₂ using the four prior model NEE fluxes is
4 shown in the right panel of Fig. 4. The most notable feature in this figure is the Northern Hemisphere seasonality, with higher
5 XCO₂ concentrations in the winter months and lowest XCO₂ values in the growing seasons of the summer. Seasonality in model-
6 predicted XCO₂ values is also evident in the TL and SL, with largest values in the autumn and lowest values in the spring. Figure
7 5 (left panel) shows the range of XCO₂ values simulated using the four prior model NEE fluxes. The differences between individual
8 model simulations of XCO₂ values deviated among themselves by up to ~10 ppm. These large differences in XCO₂ values across
9 the four different prior NEE flux models show that the choice of prior NEE has a large impact on simulated XCO₂ values.

10 **3.3 Optimized global NEE fluxes**

11 From Table 1 it can be seen that annual global mean posterior NEE flux, when using the different prior models and assimilating
12 synthetic LN+LG OCO-2 XCO₂, ranges from -4.11 to -4.36 PgC yr⁻¹, which are generally close in magnitude to the “true” flux of
13 -4.31 PgC yr⁻¹. Although these posterior NEEs generally converged to the “truth”, there are some remaining differences, with an
14 annual global mean posterior NEE range of 0.25 PgC yr⁻¹ (~6% of the multi-model-mean posterior NEE; Table 1). From the results
15 of the OSSE simulations, it was found that the spread and range in XCO₂ simulated using the optimized posterior NEE fluxes was
16 greatly reduced compared to the spread in XCO₂ simulated using prior NEE fluxes. This is evident from the right panel of Fig. 5
17 where XCO₂ simulated using posterior NEE fluxes differ among themselves by < 0.5 ppm, which is greater than an order of
18 magnitude lower, on average, than the spread among XCO₂ simulated using prior NEEs.

19 Figure 3 shows the spatial distribution of the range of prior and posterior NEEs. As expected, the range in optimized
20 posterior NEE flux estimates starting from the four separate prior models was substantially reduced compared to the spread in prior
21 NEE fluxes. However, the posterior NEE fluxes for individual surface grid boxes of the model still depict some residual range
22 among the posteriors, with the largest residuals being found across South America and South Africa in all seasons and in Temperate
23 regions of the Northern Hemisphere in the spring months. As shown in Fig. 3, the geographical pattern of the range of prior and
24 posterior NEEs does not indicate any noticeable correlations. From comparing Figs. 3 and 5, it is apparent that the spread in
25 posterior XCO₂ is significantly reduced in all regions of the globe compared to prior model simulations, however, while posterior
26 NEE values are reduced compared to the prior, noticeable residual spread remains in some regions. This emphasizes the fact that
27 the OSSEs successfully converge to match the synthetic OCO-2 XCO₂ values by optimizing NEE in different ways depending on
28 the prior NEE model used. The following sections investigate the regional differences in posterior NEE estimates due to the residual
29 impact of prior biospheric CO₂ flux predictions.

30 **3.4 Optimized regional NEE fluxes**

31 Figure 6 shows the seasonally-averaged “true”, prior and posterior NEE flux values for the 11 individual TransCom-3 land regions
32 (with detailed statistics in Table 3 and monthly-mean time-series in Fig. S6). The first thing noticed from this figure is that all
33 posterior NEE values, using variable priors, tend to reproduce the “truth” in most TransCom-3 land regions. From Fig. 6 it can
34 also be seen that the assimilation of synthetic OCO-2 LN+LG XCO₂ retrievals resulted in a large reduction in the range among the
35 four modeled NEE values (Table 3 shows the corresponding SD values). The reduction in the SD of NEE (also known as
36 uncertainty reduction) in most regions/seasons, calculated as $100 \times (1 - (\text{posterior NEE SD})/(\text{prior NEE SD}))$ is generally > 70%
37 and up to 98%. However, the range of seasonal mean posterior NEEs over individual TransCom-3 regions is still as large as 1.4
38 PgC yr⁻¹ when applying different prior NEE, with the largest ranges occurring in Northern Boreal regions (North America Boreal,

1 Eurasian Boreal and Europe) in winter months. During the spring and summer months, regions in the TL (e.g., Tropical Asia) and
2 SL (e.g., South American Temperate, South Africa) have ranges in posterior NEEs up to $\sim 0.5 \text{ PgC yr}^{-1}$. The larger residual range
3 among posterior NEE estimates for winter months in Northern Boreal regions is likely due to the insufficient OCO-2 observations
4 during this time (see Fig. 4), while the larger range in the TL and SL regions is due to differences in the priors (see Fig. 2). This
5 demonstrates that the impact from the prior model has regional and seasonal variability depending on: 1) the spatio-temporal flux
6 variabilities inherent in prior NEEs and 2) the observation density and coverage of synthetic OCO-2 data. Figure 6 and Table 3
7 show that the seasonally-averaged posterior NEE spread varies from $\sim 10\%$ to $\sim 50\%$ of the multi-model-mean for different
8 TransCom-3 land regions with significant NEE fluxes. When evaluating this residual spread in posterior NEEs on a global average,
9 seasonally-averaged values ranged from $\sim 10\%$ (JJA) to $\sim 20\%$ (DJF) of the posterior NEE mean. These statistics reveal that the
10 impact of prior models lead to a much larger spread/range for regional/seasonal posterior fluxes (up to $\sim 50\%$) compared to annual
11 global averaged values (6%). This emphasizes that while OCO-2 observations on average constrain global, hemispheric and
12 regional biospheric fluxes, noticeable residual differences in posterior NEE flux estimates remain due to the choice of prior model
13 values. Overall, the results of this evaluation suggest that when inter-comparing inverse model results assimilating similar OCO-2
14 observational data, differences in posterior NEE in regions with significant NEE fluxes could vary by up to $\sim 50\%$ when using
15 different prior flux assumptions.

16 **3.5 Impact of prior uncertainty**

17 Results of this study have demonstrated the sensitivity of posterior NEE estimates to prior NEE flux assumptions. In this section,
18 the sensitivity of posterior NEE estimates to the assumed prior uncertainty is tested, when assimilating synthetic OCO-2 LN+LG
19 XCO₂ observations. The general importance of prior uncertainty values is highlighted in the TL regions. In these regions the largest
20 differences in prior models are calculated, thus largest prior uncertainty is assigned, resulting in larger deviations from the prior
21 and posterior NEE spread similar to other TransCom-3 land regions (see Fig. 6). In order to quantify the sensitivity of posterior
22 NEE to prior uncertainty statistics, a single prior NEE flux model (CASA-GFED) is applied in the OSSE framework, with variable
23 prior flux uncertainty assumptions. Two additional OSSE simulations (in addition to the baseline simulations using the SD of the
24 four prior models as the prior uncertainty; see right panel of Fig. 2 for SD maps) are performed using prior NEE magnitudes from
25 CASA-GFED and setting the prior uncertainty uniformly as 10% and 100% of the CASA-GFED NEE values. Figure 7 shows the
26 results of these additional OSSE simulations over the TransCom-3 land regions. From this figure it can be seen that the range of
27 seasonal mean posterior NEEs over individual TransCom-3 regions vary from ~ 0.1 to $> 1 \text{ PgC yr}^{-1}$ when applying variable prior
28 error assumptions. Seasonally-averaged posterior NEE SD varies from $\sim 10\text{-}50\%$ of the multi-model-mean for different TransCom-
29 3 land regions with significant NEE fluxes. On a global average, seasonal-average SD values range from $\sim 15\%$ (JJA) to $\sim 30\%$
30 (DJF) of the posterior NEE mean. Note that these posterior NEE SD/range values here are similar to the baseline OSSEs conducted
31 by changing prior NEE flux magnitudes (see Fig. 6). However, when comparing Fig. 7 and 6 (and Fig. S7), it is noticed that
32 posterior NEE estimates are more sensitive to prior error assumptions compared to prior flux values in some seasons/regions of
33 TL and SL (e.g., Northern Africa, Southern Africa, South America Temperate). It appears that NEE estimates during this study are
34 more sensitive to prior error assumptions when sufficient observations are available and large differences between the prior and
35 “truth” are present. Also, from Fig. 7 it can be seen that prior uncertainty assumptions in the baseline runs (using SD of prior
36 models) and the assumption of 100% prior uncertainty tend to reproduce the “truth” more accurately than NEE estimates using
37 10% prior error. Overall, the results demonstrate that the posterior NEE fluxes over TransCom-3 land regions are in general
38 similarly sensitive (up to $\sim 50\%$) to the specification of prior flux uncertainties and the choice of bottom-up prior biospheric NEE
39 model estimates.

1 3.6 OCO-2 ocean data

2 This portion of the study investigates the impact of assimilating OCO-2 OG XCO₂ data on posterior NEE flux estimates in our
3 OSSE framework. To do this, four additional OSSE simulations were conducted with the four prior model NEEs when only
4 assimilating synthetic OG retrievals (instead of LN+LG) in the inversions (everything else remains the same as in the baseline
5 simulations). Figure 8 shows the results of these four additional OSSE simulations averaged over the TransCom-3 land regions.
6 From these simulations it can be seen that OCO-2 OG indeed reduces the range in posterior NEE flux estimates, when applying
7 different priors, compared to prior model predictions, and can generally reproduce the “truth”. On average, the spread in posterior
8 NEE fluxes is ~20% to ~50% of the multi-model-mean for different TransCom-3 land regions with significant NEE fluxes. As
9 expected, the comparison of Fig. 6 and 8 suggests that LN+LG data is better able to constrain biospheric CO₂ fluxes compared to
10 OG data, as the spread among the posteriors is generally lower in LN+LG only assimilations (~70% lower on a global average)
11 compared to OG data only assimilations. However, there were some cases where OSSE simulations using OCO-2 OG data alone
12 did in fact result in slightly lower posterior NEE spreads in some TransCom-3 land regions compared to LN+LG assimilations
13 runs (e.g., Northern Boreal regions during summer months and Australia during winter months). Overall, our OSSE simulations
14 using the OCO-2 OG data demonstrate the importance of these oceanic retrievals to constrain land NEE fluxes, as the posterior
15 NEE range is much lower compared to prior NEE estimates (see Fig. 8). This generally agrees with previous studies that
16 demonstrated the importance of satellite data over the ocean in constraining NEE fluxes over land regions (e.g., Deng et al., 2016).

17 4. Conclusions

18 To the best of our understanding, this is the first study directly quantifying the impact of different prior global land biosphere
19 models on the estimate of terrestrial CO₂ fluxes when assimilating OCO-2 satellite observations. We conducted a series of OSSEs
20 that assimilated synthetic OCO-2 observations applying four state-of-the-science biospheric CO₂ flux models as the prior
21 information. These controlled experiments were designed to systematically assess the impact of prior NEE fluxes and the impact
22 of prior error assumptions on “top down” NEE estimates using OCO-2 data. The OSSEs incorporated NEE fluxes from the NASA-
23 CASA, CASA-GFED, SiB-4 and LPJ biosphere models as prior estimates and variable prior flux error assumptions.

24 We found that the assimilation of synthetic OCO-2 XCO₂ retrievals resulted in posterior monthly/seasonal NEE estimates
25 that generally reproduced the assumed “true” NEE globally and regionally. However, spread in posterior NEE exists in regions
26 during seasons with poor data coverage, such as the Northern Boreal regions and some of the Tropical and Southern Hemispheric
27 regions (e.g., South American Temperate, South Africa, Tropical Asia). This spread among posterior NEEs is likely due to the
28 insufficient OCO-2 observations during winter over Northern Boreal regions and the large range among the priors in some of the
29 Northern Boreal, Tropical and Southern Hemispheric regions. Residual spread from ~10% to 50% in seasonally-averaged posterior
30 NEEs in TransCom-3 land regions with significant NEE flux were calculated due to using different prior models in inverse model
31 simulations. We also found similar spreads in the magnitudes of posterior NEEs by conducting additional OSSEs using a single
32 prior NEE flux model with variable prior flux uncertainty assumptions. While the spread in posterior NEE estimates, when using
33 variable prior error statistics, was similar to when applying variable NEE flux models, the impact was larger in some seasons in
34 the TL and SL regions. We determined that while OCO-2 observations on average constrain global, hemispheric and regional
35 biospheric fluxes, noticeable residual differences (up to ~20-30% globally and 50% regionally) in seasonally-averaged posterior
36 NEE flux estimates remain that were caused by the choice of prior model values and the specification of prior flux uncertainties.

37 There have been previous studies that investigated similar scientific objectives, such as the impact of prior uncertainties
38 on inverse model estimates of NEE (Gurney et al., 2003; Chevalier et al., 2005; Baker et al., 2006a; 2010). The sensitivity of CO₂
39 flux inversions to the specification of prior flux information was first assessed by Gurney et al. (2003) using ground-based in situ

1 data. One main conclusion from Gurney et al. (2003) is that CO₂ flux estimates were sensitive to the prior flux uncertainty over
2 regions with limited observations and insensitive over data-rich regions. Chevallier et al. (2005) suggested the importance of an
3 accurate formulation of prior flux uncertainty by conducting 4D-Var assimilation of satellite column retrievals of CO₂. Baker et
4 al. (2010) investigated the importance of assumed prior flux uncertainties by conducting sensitivity tests that mistuned the
5 assimilations by using incorrect prior flux errors. Finally, Baker et al. (2006a, 2010) suggested the need for realistic prior models
6 in the 4D-Var assimilations using OCO synthetic satellite CO₂ data. The results of this research are generally consistent with the
7 findings of these past studies. However, in comparison with these previous efforts, our study is a step forward, because we quantify
8 the specific impact of prior model NEE spatio-temporal magnitude and prior uncertainties in optimizing regional and seasonal
9 NEEs using satellite data in a more controlled manner by applying an OSSE framework.

10 As explained earlier in this study, estimates of surface CO₂ fluxes from numerous inversion systems in the OCO-2 MIP
11 ensemble model framework, using identical OCO-2 observations, result in different optimized/posterior regional NEE fluxes
12 (Crowell et al., 2019). This inverse model variance can be due to numerous factors (e.g., model transport, inversion methods,
13 observation errors, etc.) including prior model mean and uncertainty estimates. In order to estimate the amount of variance in the
14 results of posterior NEE values from the OCO-2 MIP which could be due to prior flux estimates, we compare our OSSE derived
15 residual posterior NEE range (using LN+LG) to the range in the posterior Level-4 OCO-2 Flux data (using both LN and LG)
16 (<https://www.esrl.noaa.gov/gmd/ccgg/OCO2/index.php>) in each TransCom-3 region. This comparison suggests that prior NEE and
17 uncertainty statistics could contribute 10-30% (average ~20%) of annually-averaged NEE variance calculated for each TransCom-
18 3 region in the OCO-2 Level-4 MIP flux data. Comparing this contribution of prior model impact to the OSSE study by Basu et
19 al. (2018), which calculated the impact of atmospheric transport on posterior NEE estimates when assimilating OCO-2
20 observations, this contribution is ~50% less compared to the impact of atmospheric transport. From our study and Basu et al. (2018)
21 it is estimated that the combination of prior flux/uncertainty assumptions and atmospheric transport could contribute on average
22 ~50% of the annually-averaged posterior NEE variance of the OCO-2 MIP study.

23 The results of this study suggest the need to be aware of the residual impact from prior assumptions for CO₂ global flux
24 inversions, especially for regions and times 1) where current “bottom-up” biosphere models diverge greatly and 2) without
25 sufficient observational coverage from space-borne platforms. For example, larger spread in posterior NEE estimates were
26 calculated in portions of the Northern Boreal regions that tend to have insufficient satellite data coverage and moderate differences
27 among prior biosphere models. In addition to these Northern Boreal regions, Tropical and Southern Hemispheric regions with
28 large spread among prior biosphere models, which are assigned higher prior uncertainty values resulting in largely reduced spreads
29 in posterior NEE estimates (large deviation from the prior), still have residual impact from the prior NEE predictions regardless of
30 the fact that OCO-2 data is dense in these regions. Results of this study also indicate that in some regions/seasons of the TL and
31 SL, inverse model estimates of NEE can be more sensitive to prior error statistics compared to prior flux values. Overall, in data-
32 poor regions/times, posterior estimates from inversion techniques relying on Bayesian statistics can result in similar estimates to
33 the prior flux, however, with some improvements over broader regions. Additionally, in regions/seasons where uncertainty in NEE
34 fluxes are large (e.g., in the TL where prior model NEE differences are large), inverse model estimates, applying large prior
35 uncertainty values, will still have some residual impact from the choice of prior NEE flux. Finally, care should be given when
36 interpreting flux estimates constrained with real OCO-2 satellite data over some of the regions identified in this study as it is
37 suggested here that residual differences (up to ~20-30% globally and 50% regionally) in seasonal posterior NEE flux estimates
38 can be produced by the choice of prior model values and the specification of prior flux uncertainties. Finally, the results of this
39 study suggest that multi-inverse model inter-comparison studies should consider the differences in posterior NEE flux estimates
40 caused by variable prior fluxes and error statistics used in different models.

1 **5. Code and Data Availability**

2 The forward and inverse model simulations for this work were performed using the GEOS-Chem model which is publicly available
3 at: <http://acmg.seas.harvard.edu/geos/>. The 10-sec OCO-2 data used to produce synthetic observations during this study are
4 available by request from the OCO-2 Science Team and individual OCO-2 sounding data can be downloaded here:
5 <https://oco.jpl.nasa.gov/>.

6 **6. Author Contributions**

7 SP and MJ designed the methods and experiments presented in the study and analyzed results. CP, VG, DB, KH and BP were
8 instrumental in providing biosphere model and OCO-2 data and guidance when applying these products. DH, JL and DB provided
9 components implemented in the modeling framework applied during this study. Finally, SP prepared the manuscript with
10 contributions from all listed coauthors.

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1 **Table 1: Prior and (Posterior) global annual mean NEE fluxes and CO₂ emission inventories (PgC yr⁻¹) for the year 2015 used in the**
 2 **OSSE simulations during this study.**

NEE Model	NEE flux (PgC yr⁻¹)
MsTMIP ^{1,2}	-4.31
NASA-CASA ³	-1.86 (-4.14)
CASA-GFED ⁴	-2.42 (-4.24)
SiB-4 ⁵	0.95 (-4.11)
LPJ ⁶	-5.53 (-4.36)
Inventory	CO₂ emission (PgC yr⁻¹)
Fossil fuel ⁷	9.86
Ocean ⁸	-2.41
Biomass burning ⁹	2.05
Fuel wood burning ⁹	0.50

3 ¹MsTMIP NEE dataset is representative of the year 2010 and is an ensemble mean of 15 different NEE models.

4 ²Huntzinger et al., 2013; 2016; Fisher et al., 2016a,2016b

5 ³Potter et al., 1993; 2012a; 2012b

6 ⁴Potter et al., 1993; Randerson et al., 1996

7 ⁵Haynes et al., 2013; Baker et al., 2013

8 ⁶Sitch et al., 2003; Poulter et al., 2014

9 ⁷Oda et al., 2018; Nassar et al., 2013

10 ⁸CarbonTracker CT2016; Peters et al., 2007

11 ⁹CASA-GFED3; van der Werf et al., 2004; 2006; 2010

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1 **Table 2: Summary of the different OSSEs conducted during this work.**

Experiment (# of OSSEs)	OCO-2 XCO₂ Mode	Prior NEE Model	NEE Uncertainty
Variable Prior NEE (4)	LN + LG	All ¹	Multi-Model SD ²
Variable Prior NEE (4)	OG	All ¹	Multi-Model SD ²
Variable Prior Uncert. (2)	LN + LG	CASA-GFED	Uniform 10%/100%

2 ¹ NASA-CASA, CASA-GFED, SiB-4 and LPJ

3 ² SD = standard deviation

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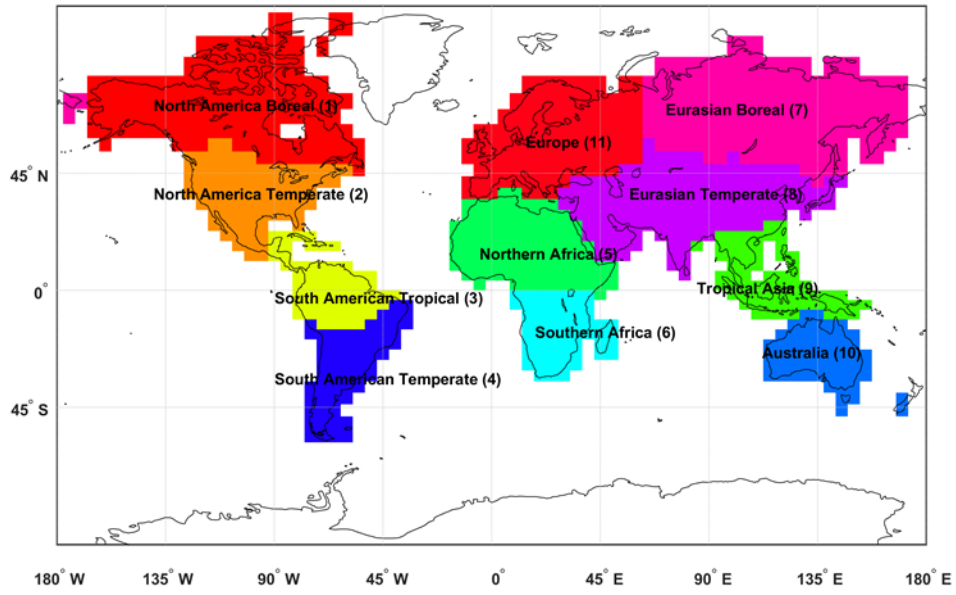
1 Table 3: Data corresponding to Fig. 6. Seasonally-averaged NEE (PgC yr⁻¹) averaged over the 11 TransCom-3 land regions (refer to Fig.
 2 1) for the MsTMIP (“truth”), multi-model prior mean and multi-model posterior mean (PgC yr⁻¹). The differences between the prior
 3 and posterior model NEE values are presented as SD (1σ) and range. Prior model values are presented in standard font and posterior
 4 estimates are in bold. Seasons are represented as Winter (W): December-February, Spring (Sp): March-May, Summer (Su): June-
 5 August and Fall (F): September-November. The synthetic observations in these OSSE simulations correspond to the OCO-2 LN+LG
 6 observing modes.

Region*	NEE: Truth				NEE: Mean				NEE: Standard Deviation				NEE: Range															
	W	Sp	Su	F	W	Sp	Su	F	W	Sp	Su	F	W	Sp	Su	F												
1	1.1	-0.2	-2.8	0.7	1.1	1.0	0.4	0.3	-3.4	-2.7	1.3	0.9	0.5	0.4	0.5	0.1	0.8	0.2	0.5	0.1	1.2	0.9	1.0	0.3	1.9	0.5	1.2	0.2
2	1.5	-1.5	-2.3	0.0	1.9	1.6	-1.0	-1.6	-3.2	-2.1	0.6	-0.2	1.1	0.3	1.3	0.1	2.0	0.2	0.8	0.1	2.3	0.6	3.2	0.2	4.3	0.4	1.6	0.2
3	-0.6	-0.2	-1.4	-1.3	0.4	-0.8	0.6	0.2	-0.7	-1.2	0.1	-1.3	0.1	0.1	0.8	0.2	1.4	0.0	2.6	0.1	0.2	0.1	1.8	0.3	3.1	0.1	5.9	0.2
4	-1.5	-0.4	0.7	-0.4	-1.1	-1.3	-0.1	-0.4	0.6	0.7	0.0	-0.1	0.9	0.1	0.4	0.2	0.8	0.1	0.9	0.1	2.0	0.1	0.9	0.5	1.9	0.2	2.0	0.3
5	1.3	1.0	-1.9	-2.0	0.7	0.9	0.6	0.4	-0.8	-1.7	-1.4	-2.0	1.0	0.2	0.8	0.1	0.9	0.1	1.2	0.2	2.3	0.5	1.6	0.3	2.0	0.2	3.0	0.5
6	-2.4	-1.6	1.2	1.2	-0.9	-1.9	-1.1	-1.8	0.3	0.8	0.7	1.2	0.5	0.2	1.0	0.1	1.2	0.2	0.7	0.1	1.2	0.3	2.2	0.2	2.6	0.5	1.7	0.2
7	1.2	1.0	-4.6	1.2	1.5	1.2	0.9	0.9	-5.6	-4.8	2.0	1.3	0.9	0.7	1.0	0.1	1.6	0.1	0.6	0.2	1.8	1.4	2.2	0.3	3.3	0.2	1.3	0.6
8	1.4	0.0	-1.9	-0.4	1.4	1.3	-1.0	-0.2	-2.3	-2.3	0.1	-0.7	1.3	0.3	0.9	0.1	2.5	0.2	1.7	0.1	3.0	0.6	2.1	0.3	5.7	0.5	3.7	0.2
9	-0.1	0.4	-0.3	-0.5	0.1	0.3	0.0	0.6	-0.4	0.1	-0.5	-0.4	0.4	0.2	0.4	0.1	0.4	0.3	0.8	0.0	0.8	0.5	0.7	0.2	0.8	0.5	1.9	0.1
10	-0.6	-0.6	-0.2	-0.7	-0.1	-0.6	0.0	-0.7	0.1	-0.4	-0.1	-0.8	0.4	0.1	0.3	0.1	0.3	0.1	0.6	0.1	0.9	0.2	0.6	0.2	0.7	0.3	1.2	0.3
11	2.8	-1.7	-3.2	1.6	2.3	2.6	-0.9	-1.2	-3.7	-3.1	1.6	1.3	0.4	0.6	1.2	0.2	1.5	0.1	0.6	0.1	0.9	1.3	2.5	0.5	3.5	0.3	1.5	0.3

*TransCom-3 region name and location displayed in Fig. 1.

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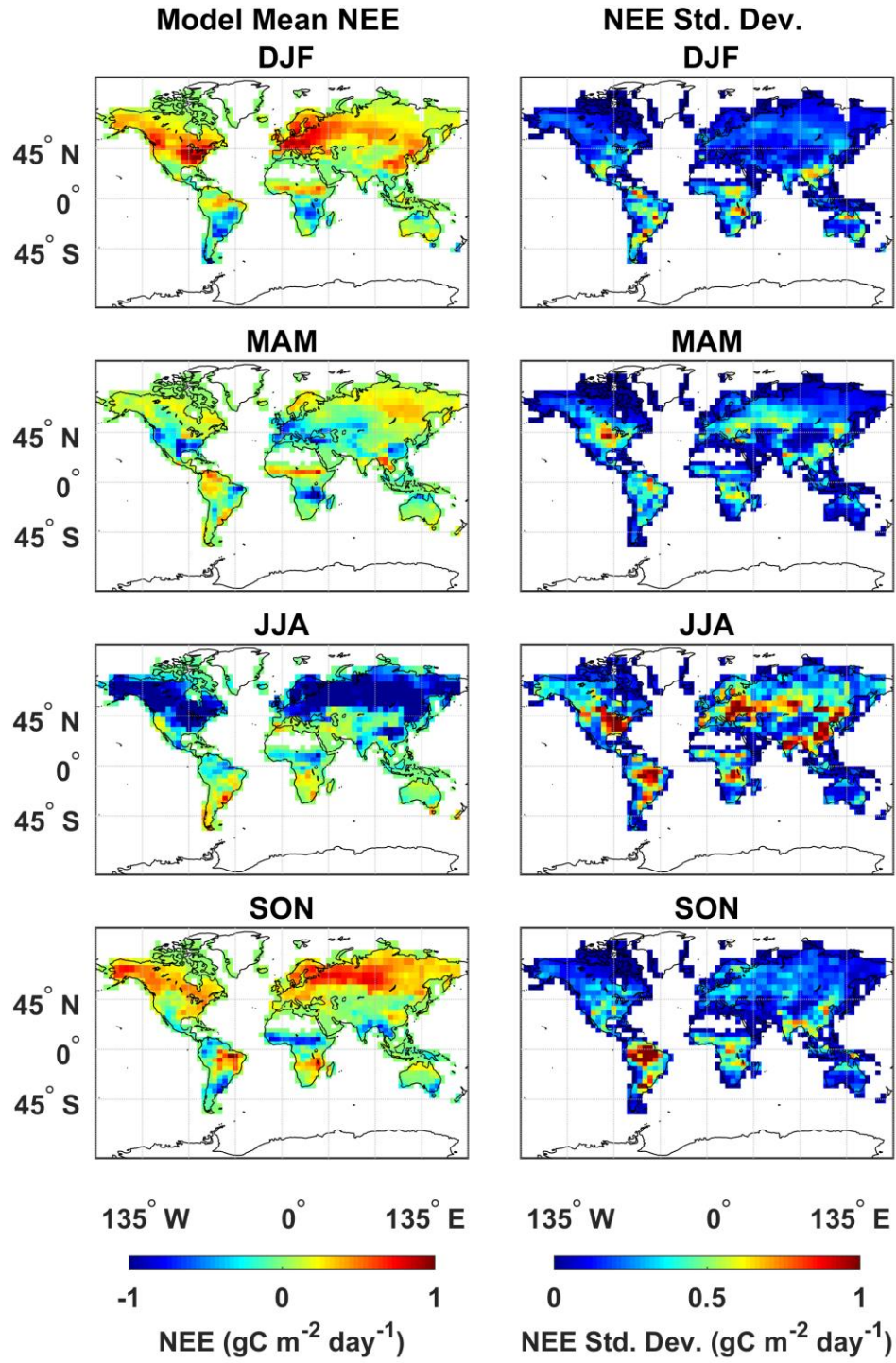
TransCom-3 Land Regions



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2 **Figure 1: The TransCom-3 land region boundaries used to aggregate CO₂ fluxes for evaluation.**

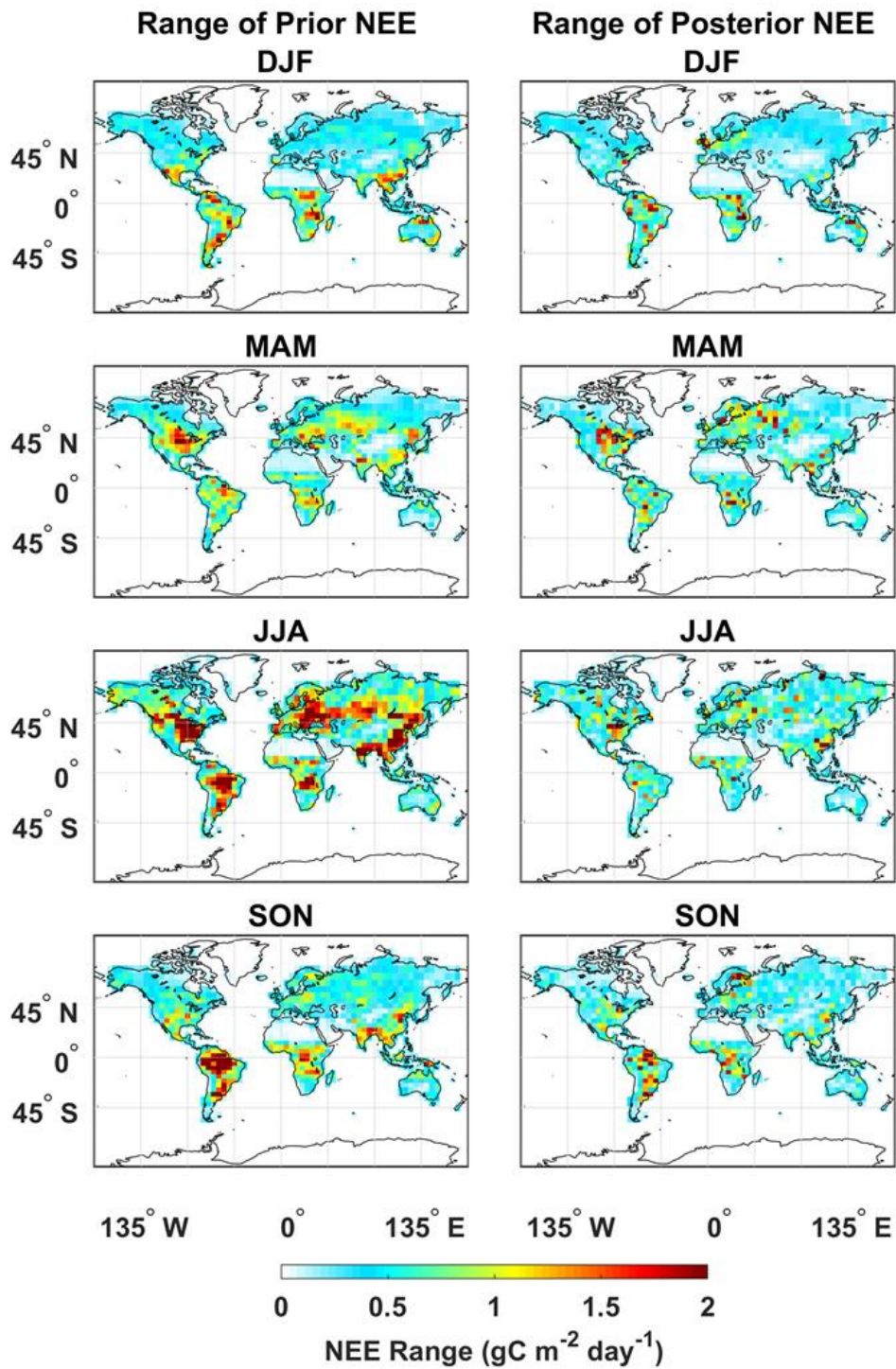
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3 **Figure 2:** Prior multi-model (NASA-CASA, CASA-GFED, SiB-4 and LPJ biosphere models) seasonally-averaged NEE ($\text{gC m}^{-2} \text{ day}^{-1}$)
4 (left column) and NEE standard deviation ($\text{gC m}^{-2} \text{ day}^{-1}$) (right column) for the year 2015.

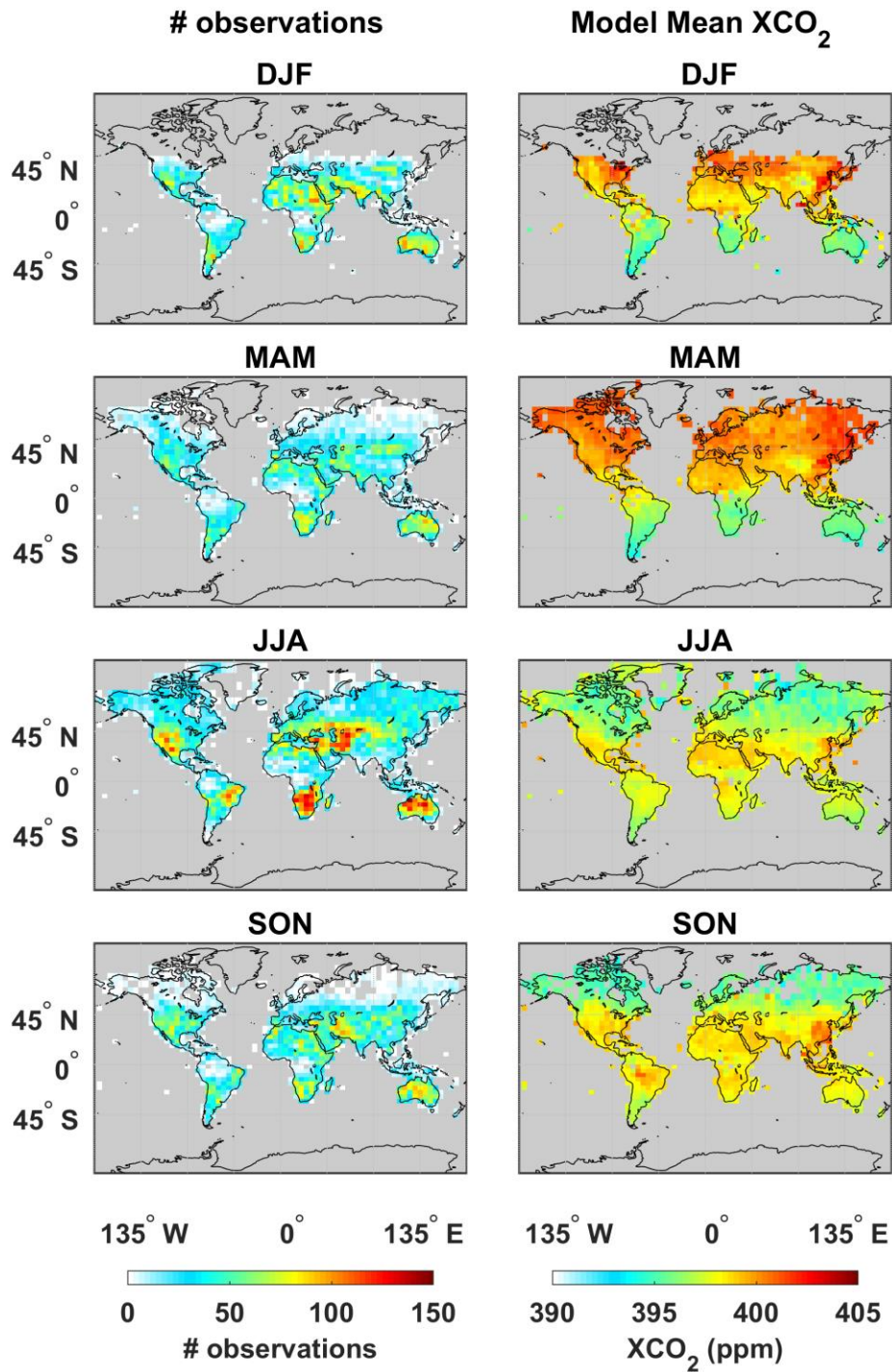
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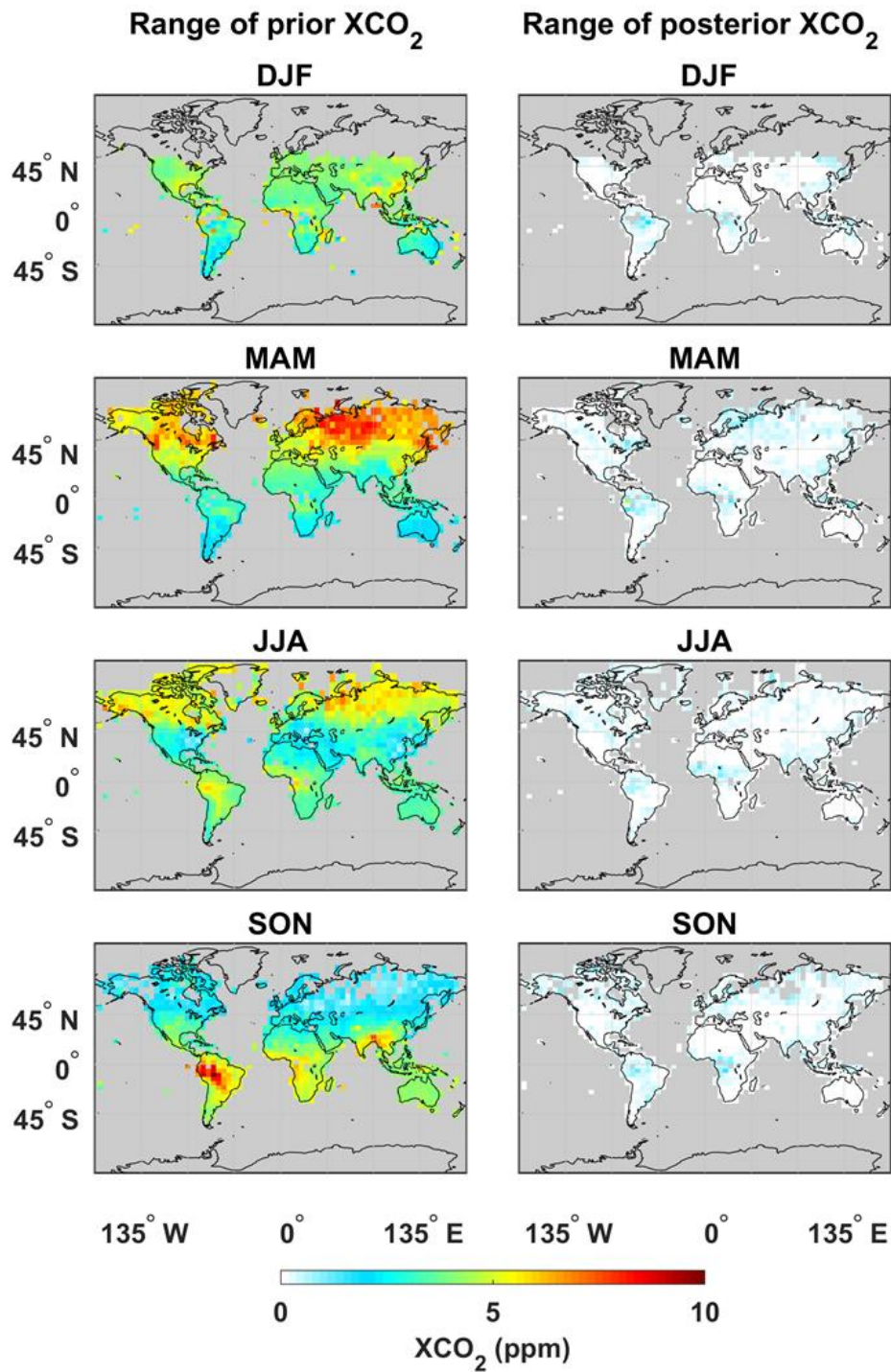
2 **Figure 3: Seasonally-averaged NEE range ($\text{gC m}^{-2} \text{ day}^{-1}$) of the four prior biosphere models (NASA-CASA, CASA-GFED, SiB-4 and**
 3 **LPJ) (left) and posterior estimates (right) from the OSSE simulations. The synthetic observations in these OSSE simulations correspond**
 4 **to the OCO-2 LN+LG observing modes.**

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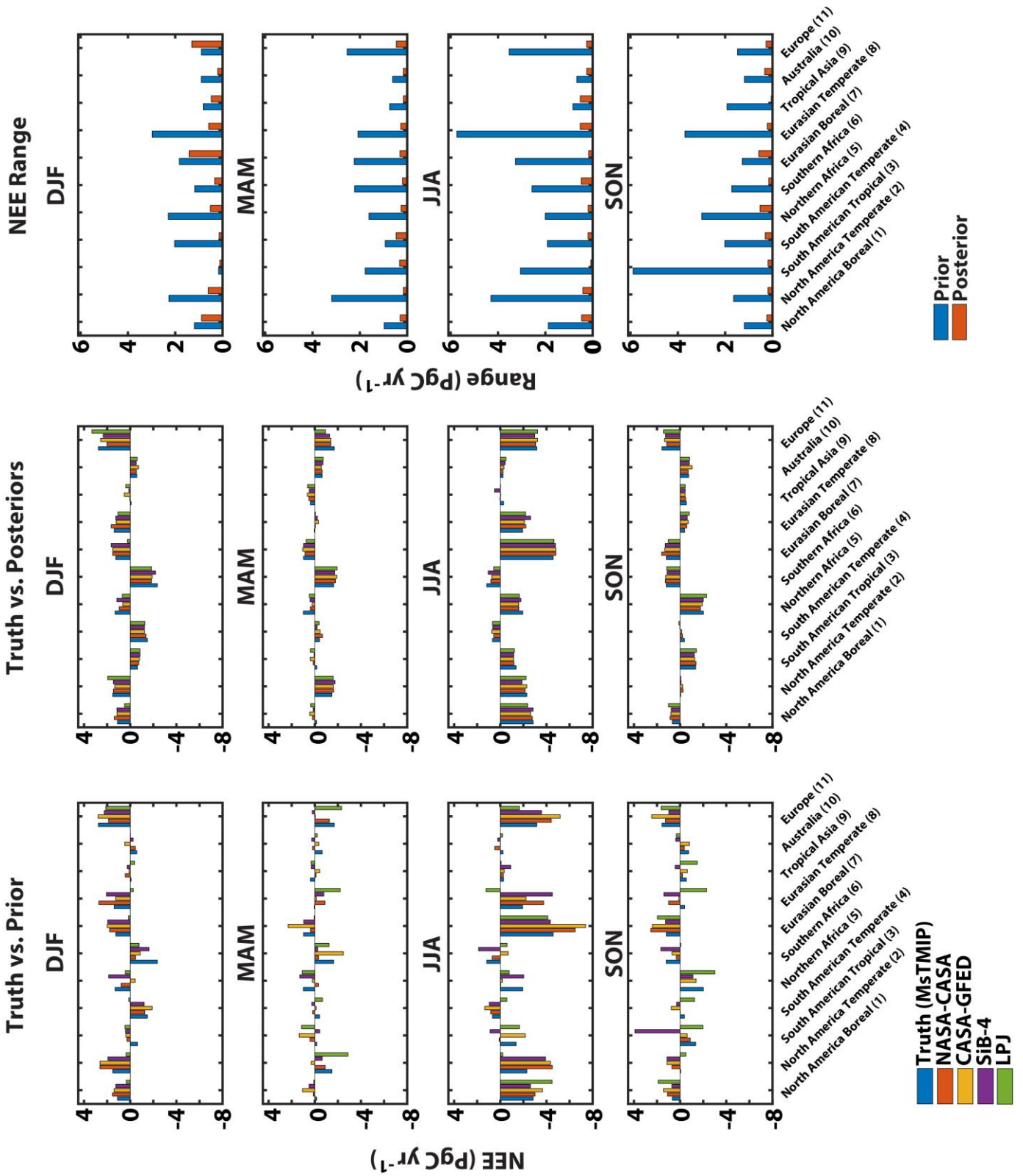
Figure 4: Total number of OCO-2 LN and LG XCO₂ observations (left column) and the corresponding seasonally-averaged multi-model (NASA-CASA, CASA-GFED, SiB-4 and LPJ biosphere models) mean GEOS-Chem-simulated prior XCO₂ (ppm) (right column) in 2015.



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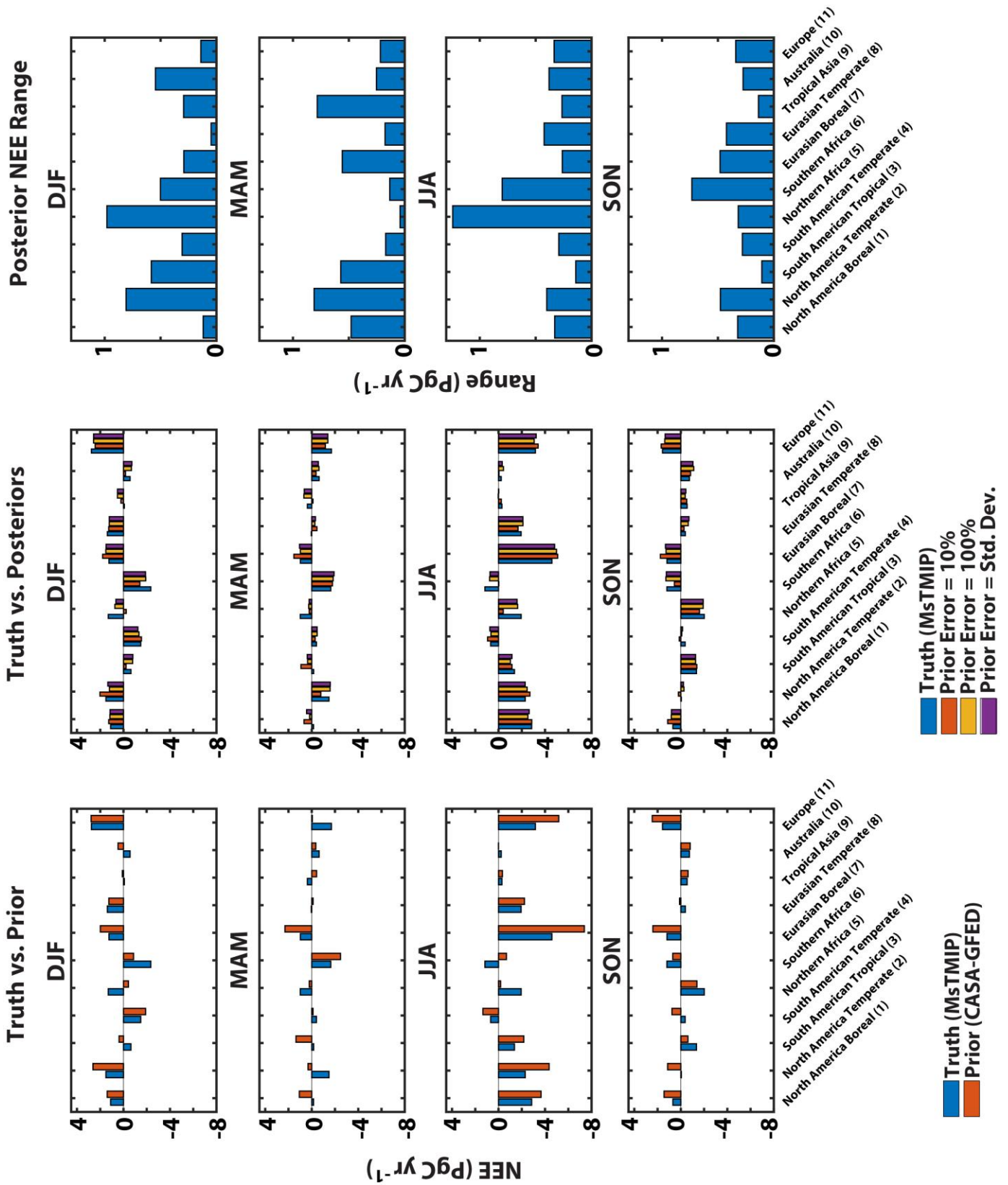
2 **Figure 5: Seasonally-averaged XCO₂ range (ppm) from GEOS-Chem forward model simulations using the four prior biosphere models**
 3 **(NASA-CASA, CASA-GFED, SiB-4 and LPJ) (left) and the corresponding posterior estimates (right) from the OSSE simulations. The**
 4 **synthetic observations in these OSSE simulations correspond to the OCO-2 LN+LG observing modes.**

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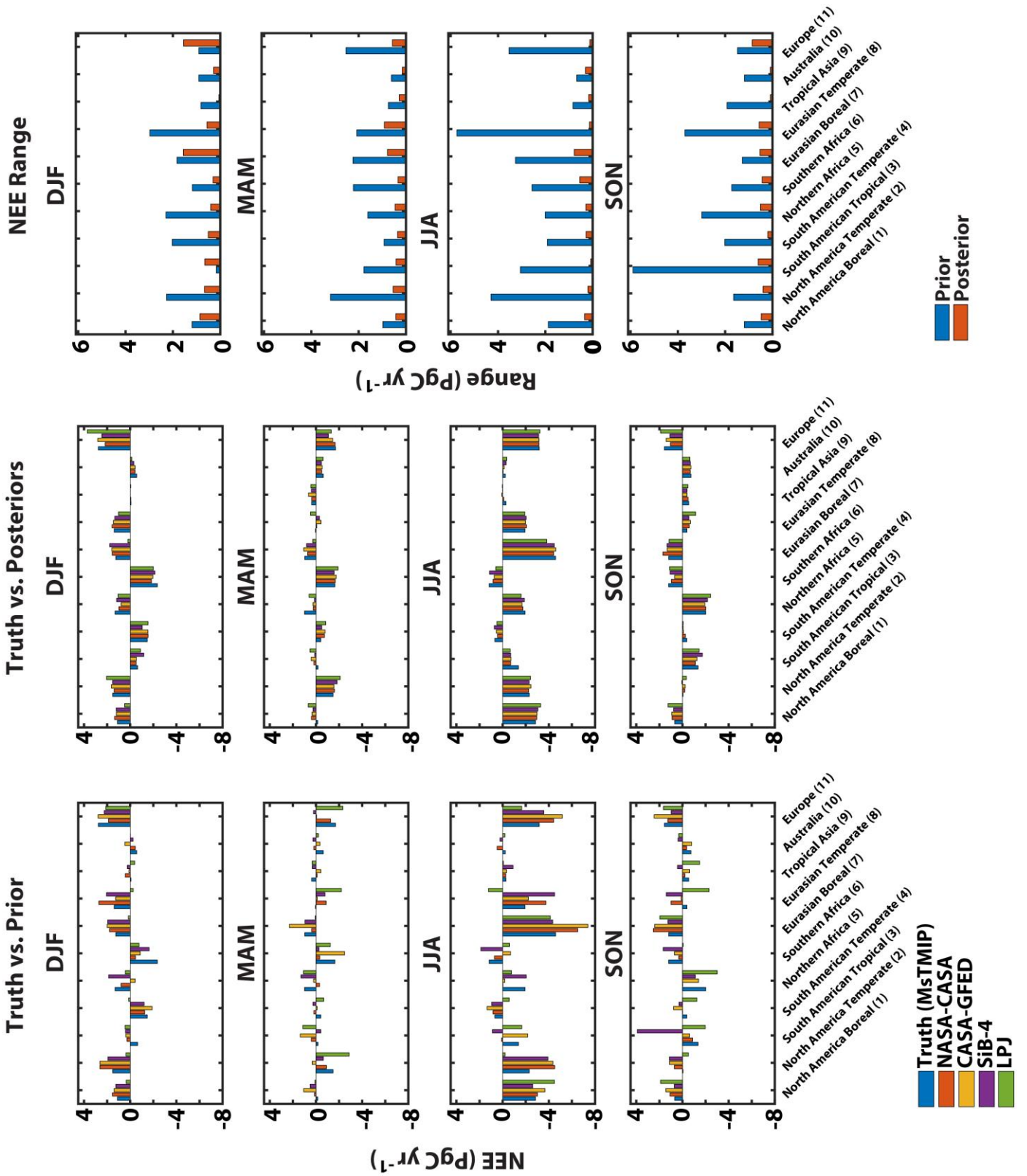
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Figure 6: Seasonally-averaged NEE (PgC yr^{-1}) averaged over the 11 TransCom-3 land regions from MsTMIP (“truth”) versus the prior biosphere models (NASA-CASA, CASA-GFED, SiB-4 and LPJ) (left column), posterior estimates (middle column) from the OSSE simulations and the corresponding range of prior and posterior NEE estimates (right column). The synthetic observations in these OSSE simulations correspond to the OCO-2 LN+LG observing modes. Detailed statistics of the “truth”, multi-model means of prior and posterior NEE estimates, standard deviations, and ranges displayed in this figure are listed in Table 3.



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Figure 7: Seasonally-averaged NEE (PgC yr^{-1}) averaged over the 11 TransCom-3 land regions from MsTMIP (“truth”) versus CASA-GFED prior biosphere model (left column), posterior estimates with the three different prior uncertainties (middle column) and the corresponding range of posterior NEE (right column). The synthetic observations in OSSE simulations correspond to the OCO-2 LN+LG observing modes. Detailed statistics of the “truth”, prior, multi-model mean of posterior NEE estimates, standard deviations, and ranges displayed in this figure are listed in Table S1.



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Figure 8: Seasonally-averaged NEE (PgC yr^{-1}) averaged over the 11 TransCom-3 land regions from MsTMIP (“truth”) versus the prior biosphere models (NASA-CASA, CASA-GFED, SiB-4 and LPJ) (left column), posterior estimates (middle column) from the OSSE simulations and the corresponding range of prior and posterior NEE (right column). The synthetic observations in these OSSE simulations correspond to the OCO-2 OG observing mode. Detailed statistics of the “truth”, multi-model means of prior and posterior NEE estimates, standard deviations, and ranges displayed in this figure are listed in Table S2.