Response to reviewers: ACP-2021-16

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This document presents a point-by-point reply to the reviewer comments on manuscript ACP-2021-16 (entitled "Was Australia a sink or source of CO_2 in 2015? Data assimilation using OCO-2 satellite measurements"). This reply is written on behalf of all co-authors.

We would like to thank the reviewer for their comments and efforts towards improving our manuscript. The reviewer's comments are given in Roman type, and our replies are shown in blue.

1 Response to referee #1

Interactive comment on "Was Australia a sink or source of CO_2 in 2015? Data assimilation using OCO-2 satellite measurements" by Yohanna Villalobos et al.

The manuscript by Villalobos et al. (2021) evaluates terrestrial biosphere carbon dioxide (CO_2) fluxes in Australia for the year 2015. This analysis was conducted with a regionalscale inverse modeling framework which assimilated Orbiting Carbon Observatory-2 (OCO-2) retrievals of column-averaged CO_2 (XCO2). The main result of the study was the larger biospheric uptake of CO_2 in Australia during 2015 compared to years prior. The study suggests that the main biomes causing this larger update were the northern savannas, Mediterranean regions, and sparsely vegetative areas. Additional information is evaluated to suggest processes which caused these anomalous fluxes. The article is relatively well-written, results are novel and presented effectively, and overall conclusions are interesting. This study is also commendable in the fact it addresses an increasingly important frontier for using OCO-2 retrievals to derive sub-regional biospheric CO_2 fluxes. The study design and results are appropriate for the journal; however, in the current form, I can not recommend this paper for publication in Atmospheric Chemistry and Physics (ACP). As described in the comments below, many key features in the observations and modeling framework, which could have significant impact on the model results, are not described/evaluated in sufficient detail. It is a concern of the reviewer that these oversights could have influenced the model results which is heavily relied on in this study. I do however feel that if the authors can sufficiently address the major comments presented here that it could potentially be published in ACP in the future.

Minor Comments

- 1. Line 7. "the Mediterranean ecotype" instead of "Mediterranean".
- 2. Line 12. "concentrations".
- 3. Line 29. "(CO2)".
- 4. Line 48. "to the period".
- 5. Line 110-111. "Haverd et al. (2020) ran...".
- 6. Line 267. I think the authors want to refer to Fig. A1.
- 7. Figure 6. Please use the same y-axis values for all figure panels to avoid any unnecessary confusion.

All the minor comments have been corrected in the manuscript.

Major comments

1. To help provide some background/estimate about the uncertainty of global inverse model estimates of biospheric CO_2 fluxes in Australia when assimilating satellite and in situ data, in addition to the text provided already in the introduction section of this study, the authors could access gridded results of the version 9 OCO-2 Multi-model Intercomparison Project (MIP) (https://www.esrl.noaa.gov/gmd/ ccgg/0C02_v9mip/index.php). This data set provides prior and posterior estimates of Net Biome Exchange (NBE) from up to 10 global models for the four-year interval of 2015-2018. This data set could have also been used to further compare to, and evaluate, some of the results of this study. This study does compare the results to 5 global inverse models. However, the OCO-2 MIP is a controlled experiment which can help with interpreting results due to specific processes (e.g., transport model, spatial resolution, a prior fluxes, observation modes, etc.). One thing that should be taken into consideration, which has been demonstrated with OCO-2 MIP results, is that notable differences in terrestrial carbon flux estimates are derived depending on which transport model (e.g., GEOS-Chem or TM5) is used for the inversion. Using a single transport model (i.e., WRF) could result in biased biospheric CO_2 fluxes simply due to a specific model's transport errors. Using a model ensemble, such as that derived by the v9 OCO-2 MIP, can help better understand these potential biases. This is just a suggestion to the authors to provide a data set to help interpret results of this study and should not be considered a requirement for application here.

We thank the reviewer for their suggestion. We compared our results with OCO2 Multi-model Intercomparison Project (MIP). This dataset has been valuable for us to evaluate our posterior fluxes further and provide more confidence in our findings.

The analysis of the ensemble annual mean of MIP-OCO2 global inversion suggests that the carbon budget for Australia was -0.17 ± 0.53 PgC y⁻¹ compared to our posterior estimate $(-0.30 \pm 0.09 \text{ PgC y}^{-1})$ (Fig. 1, in this revision document). We can see in Fig. 1 that the seasonal pattern between MIP ensemble mean flux and our posterior carbon fluxes are quite similar, and both estimates fall within 1-sigma uncertainty. July is one exception to this agreement with a posterior flux of -1.71 ± 0.39 PgC y⁻¹ compared to the MIP ensemble mean (-0.33 \pm 0.53 PgC y⁻¹). Analysing the spatial distribution of these two carbon flux estimates, we found that the distribution of the MIP ensemble mean in July is similar to our posterior fluxes (both carbon sinks are located in southeastern Australia). However, the magnitude of our posterior sink is stronger compared to the MIP ensemble mean (see Fig 2(g) and Fig. 3(g)). To further analyse our results, we also assess how well our posterior monthly spatial maps agree with these ten global inversions individually. We plotted monthly maps for each global inversion (see appendix of this document). Looking at the monthly spatial maps of these global inversions for 2015, we found that our posterior flux distribution across Australia agree well with at least five global inversions (TM5, CAMS, PCTM, LoFi AMES). We believe that this intercomparison is valuable for Australia because it shows that our results are reliable with a better spatial resolution than global inversion. We will include these results in the discussion section of our manuscript, and I will contact all the OCO-2 MIP modelling group before submitting the final version of the paper to the Journal.



Figure 1: Dot grey point in (a) shows the ensemble annual mean of ten MIP-OCO2 global inversion (AMES, PCTM, CAMS, CMS-Flux, CSU, CT, LoFI, OU, TM5-4DVAR, UT) for 2015. The error bar in this graph shows the spread of these models. The orange and blue points show the annual mean of the prior and posterior biosphere land CO_2 flux associated with its uncertainties (Note that the posterior uncertainties in this study were calculated by OSSEs). The grey dots in (b) show the ensemble monthly mean of the ten global inversions described in (a), and the error bars represent the monthly mean spread of this models. The orange and blue points in (b) represent the prior and posterior flux estimated (All fluxes in this comparison are without fossil fuel emissions.



Figure 2: Posterior fluxes using assimilated data from OCO-2 observations observations (land nadir and land glint data for 2015).



Figure 3: OCO-2 MIP posterior ensemble mean using assimilated data from OCO-2 observations (land nadir and land glint data for 2015).

2. The authors state they use "fixed patterns" for initial and boundary conditions and then solve for scaling factors. Can more detail be provided about this? Boundary conditions can be very important for the accuracy of regional-scale inversion estimates for long-lived species. First, how large is the domain used in this study? This information would be good to present to the reader prior to discussing the boundary conditions. Are the boundary conditions provided as daily, monthly, seasonal, or annual averages? Are the scaling factors derived hourly or daily to reflect variability in the boundary conditions of CO₂? It is difficult to understand what exactly the authors did for this. Also, what is meant by the upper and lower areas of each quadrant? Please provide actual altitude or pressure levels which separate these areas. It would be very helpful if the authors could provide some information about the sensitivity of the results of this study to the boundary conditions used in the modeling framework.

We agree with the reviewer that regional inversions are sensitive to boundary conditions. We evaluated the impact of adding bias in the boundary conditions (BCs) in Villalobos et al. (2020). In this study, we increase BCs of the CMAQ model domain by adding a constant offset of 0.5 ppm on each grid cell. We showed that our inversion system was able to correct the biases incorporated in our system. We believe that it is not necessary to perform another sensitivity case. We also agree that a better explanation of how our system handles the BCs is important for the reader. The following text will be included in the manuscript:

BCs are incorporated to the control vector $\vec{x} = \{i_0, e_0, e_1, ..., e_n, b_0, ..., b7\}$ as eight boundary regions $b_0, ..., b7$ (representing the upper and lower areas of the North, South, East and West sides of the rectangular domain) (Fig. 2 shows the boundary lateral component and the domain in our study case). The lower BCs regions cover eight layers of the atmosphere (sigma level 1 up to 0.96), which correspond (on average) to a pressure of 972.5 hPa, and upper BCs regions cover the other 12 CMAQ vertical layers (up to 50 hPa). Our system solves for these boundary lateral components (which we call fix patterns), while surface fluxes are also being optimized. Boundary conditions are provided to the CMAQ model as daily averages, but we optimize them as monthly averages.

As mentioned in the manuscript, the CMAQ model can ingest 3-dimensional emissions so we treat the unknowns related to the BCs as scaling factors for these emissions. We calculate their magnitudes from concentration tendencies in the CAMS data.



Figure 4: Representation of the horizontal WRF (black rectangle) and CMAQ model domain (red rectangle). Boundary components (south, east, north and west) are represented as blue rectangles. Land biosphere emissions incorporated over Australia are represented by the small red rectangle (CABLE model in BIOS-3 set up). Outside this area, land biosphere emissions come from CABLE global product.

3. It sounds as if the prior biospheric CO₂ model fluxes did not cover the entire domain investigated in this study. Once again, it would be helpful for the reader to know the domain dimensions prior to this discussion. For the areas not covered by the BIOS3 product the authors incorporated monthly biosphere fluxes from Australia CABLE-POP global simulations. What spatial resolution is the global model provided at? How different are the global CABLE-POP results to the fluxes derived from the BIOS3 product?

Our study domain covers the Australia region and other countries such as New Zealand, Indonesia and Papúa New Guinea (See Fig. 2). We extended our domain to minimize the influence of the exterior boundary conditions. CABLE model runs in the BIOS-3 setup rely on their regional driver and observations, which do not exist outside the domain of the Australian continent. These data (BIOS-3) provide the advantage of the best possible prior for Australia. Land areas that are not covered by CABLE BIOS-3 simulations were derived using CABLE-POP global runs (runs included in TRENDY intercomparison version 8). The spatial resolution of this global product were given at 1 degree compared to CABLE BIOS-3, which was given at 0.25 degree.

4. Why did the authors decide to exclude small fires in their prior biomass burning emission inventory? The authors should provide some reasoning for this. Do small fires not contribute much to the overall biomass burning emission total for Australia? How were the GFED emissions scaled to an hourly resolution? Also, are biofuel emissions considered in the prior CO₂ flux estimate?.

We did not exclude fires emission from GFED product, because we used the fourth version of the Global Fire Emissions Database (GFED 4.1s). We forgot to update this information in the manuscript. We will correct the text which says that GFED emissions were scaled to an hourly resolution because we assumed GFED was constant across the months, and we did not include biofuel emissions in the prior flux estimate.

5. The description of how prior flux error/uncertainty estimates for all flux sources is missing. Also, what flux sources are constrained in the CMAQ simulations? Are all CO₂ sources and sinks allowed to be adjusted when assimilating OCO-2 data? What spatial and temporal resolution are these flux constraints calculated at? Does the domain include oceanic regions? Are these ocean fluxes allow to be adjusted? Given that Australia is both upwind and downwind of oceanic regions, these emission fluxes will have a large impact on XCO2 values over the Australian continent. This needs to be described in more detail. In the results section the authors do state that they "do not allow much freedom for ocean fluxes" implying that ocean flux prior uncertainties were set to be small values. This could greatly impact posterior land flux estimates due to the fact Australia's XCO2 values will be significantly impacted by ocean fluxes.

We agree with the author that a better description of the prior and uncertainties should have been provided in the document. We did not include much detail of them, because a complete description of prior characterization was made in Villalobos et al. (2020). The text in section 2.3 in this manuscript will be updated with more details about how we construct the prior and their uncertainties. Regarding the reviewer's questions, we constrain anthropogenic fluxes, fires, land and ocean fluxes in the CMAQ simulations, and all of them were adjusted by the optimizer when assimilating OCO-2 data. We solve for monthly averaged fluxes at the CMAQ horizontal grid-resolution (81 km). Our study domain as seen in Fig. 2 includes ocean regions. Emissions over ocean were taken from the latest version of CAMS greenhouse inversion (Chevallier, 2019). We did adjust ocean fluxes, but not much (this is because our prior error covariance matrix was decomposed along its eigenvectors and eigenvalues, where most of the variance was capture over land). We did not give much flexibility to inversion to move ocean fluxes because the ocean uncertainties were assumed to be small in comparison with emission uncertainties over land.

6. Details about how the observational error/uncertainty matrix was calculated (e.g., transport error, model-data mismatch, etc.) needs to be described as well. Are individual soundings of OCO-2 retrievals used for comparison to the model, or is there some temporal/spatial averaging? The authors point to a past study for these methods, but the way OCO-2 data is treated in this study is important enough to be presented in this manuscript.

We will describe with more details in the manuscript how we calculate the error covariance matrix for the observations. With regards to the reviewer's questions, we averaged all the OCO-2 soundings for comparison to the CMAQ model followed the advise of David F. Baker (personal communication). To construct this average, we used a two-step process, first we grouped OCO-2 sounding across 1-second spans, then we grouped those across 11-second spans. This averaging procedure is similar to the one used by Crowell et al. (2019).

7. How do the authors extrapolate the vertical CO₂ profile in CMAQ above 50 mb? Will some of the offset in the model-data XCO2 comparison be due to the fact the model does not account of this part of the vertical profile? Satellites (e.g., OCO-2, GOSAT) have sensitivity to this stratospheric CO₂ and will contribute to the overall retrieved XCO2 values.

We did not extrapolate the CMAQ vertical CO_2 profile above 50 hPa. We assigned everything above the model-top (50 hPa) to the top layer of the model, which only represents 5% of the mass of the atmosphere. In order to assess how much impact this assumption would have in the model-data XCO2 comparison, we made a simple extra comparison where we assumed that the CMAQ XCO2 column-average concentration derived from our interpolation only accounts for 95% mass of the atmosphere, and the rest (5%) corresponds to the upper model-top concentration in the CMAQ model. We found that the difference between "the model-data XCO2 comparison" and this simple extra comparison was minimal, and on average, for the whole CMAQ domain, this difference only represents about 0.03 ppm. These findings were expected because the vertical profile variation above 20 km shows less variability than below this height.

8. A major result presented by the authors is that "either prior uncertainties or observational uncertainties were too high" in the model setup used in this study. Can the results of the posterior fluxes be trusted due to this? Just because the posterior CO_2 concentrations compare better to the observations, compared to the prior, does in

no way mean that the posterior fluxes are more accurate. The authors need to expand upon this and provide evidence of why the posterior fluxes are realistic.

We meant to say on page 1.3 in the manuscript that either the prior or observation were too low in the model set-up. We understand the concern of the reviewer related to the prior and observational uncertainties. On page 10 (section 3.1 of the manuscript), we indeed stated that the cost function and observation ratio was not 0.5, as we expected (but it was close to one). We thought that such a slight difference might potentially have a relatively small impact on the final fluxes. To assess this claim, we ran a sensitivity experiment in which we increased both the prior and observations uncertainties by a factor of 1.2. Preliminary results showed that after 20 iterations, our system reaches the expected theoretical value. The analysis of the convergence shows the ratio between the observations (9556.0) and the final cost function (4427.0) is 0.46 (close to 0.5). We found that our monthly posterior fluxes did not change much compared to the previous run and provide evidence that our posterior fluxes are realistic. These results will be included in the new version of the manuscript.

9. When the authors compare monthly and annual terrestrial CO₂ fluxes, do these include biomass burning emissions? Were fires anomalous in 2015 compared to prior years? Were the fires adjusted significantly due to the assimilation of OCO-2 observations? This is an important point because if prior fire emissions are not treated correctly in the inversion, and the fires were significant different during this year, the inversion could bias the land sink high or low. Something similar could be said for oceanic fluxes. The authors should present values, and spatial maps, for the source attribution of prior and posterior CO₂ fluxes for the domain. Since the description about what fluxes were constrained in the inversion, and how the individual source prior errors were attributed, it is difficult to understand and trust the results of the study.

We cannot determine if the fires were adjusted significantly due to the assimilation of OCO-2 observations because we did not solve for the fire flux separately. We solve for the net flux, which includes fires, fossil fuel and land emissions. To answer the review question relating to anomalies fires in 2015, we calculate the GFED fire anomalies for 2015 relative to the mean 2000–2014. Fig. 6 shows that fires that occurred in April, May and November in the northern region of Australia were anomalous for Australia. We will include these spatial maps in the manuscript and the source attribution of prior and posterior CO_2 fluxes for the Australia domain.



Figure 5: Fires fluxes for 2015 derived from GFED4s.



Figure 6: Fire flux anomalies in 2015 (relative to the mean 2000-2014).

10. Are the 0-50 mm rainfall anomalies for southeast Australia in July 2015 significant? What is the fractional increase in rainfall for this region this equates to? There are regions of Australia in the same year that received up to 700 mm more rainfall in a respective month. Also, depending on when the rainfall was occurring in July, it might not even have much effect on the EVI values and could be impacted by months prior. It appears June 2015 had a slightly higher anomaly in rainfall in the same region. The authors are quick to attribute the increase in biospheric carbon uptake to increased EVI and rainfall, which may be true, but more analysis/explanation would help.

We plotted the fractional increase of rainfall per grid-cell for the whole of Australia for 2015 (relative to mean 2000–2014) (see Fig. 7). We found that about 50 mm in southeast Australia in July 2015 represents about 60% of a increase of rainfall (relative to mean 2000-2014). To a certain extent we agree with the reviewer that the rainfall anomalies across southern-east Australia in May and June (previous to July) also contributing to increase in vegetation in this region. However during wet times in this region, pasture may grow quickly and become dense.



Figure 7: Rainfall anomalies for 2015 (relative the mean 2000–2014).



Figure 8: Percentage of increase in rainfall for 2015 (relative the mean 2000–2014).

11. What data is used to derive the six bioclimatic classes used in this study? The authors point to a past study, but the information is needed here.

The six bioclimatic classes used in this study correspond to an aggregation of the 18 agro-climatic zones generated by Hutchinson et al. (2005). The climatic classification in Hutchinson et al. (2005) was adapted from an existing global agro-climate classification (Hutchinson, 1992), which was refined and closely aligned with natural vegetation formations and common land uses across Australia using 182 weather climate stations and the Interim Biogeographic Regionalisation for Australia (IBRA).

12. One of the most striking and surprising results is the large increase in carbon uptake in the sparsely vegetated (mainly desert) region of Australia. The authors state this "might be associated with an underestimation of the GPP by CABLE-BIOS3". This is true of course, but why would a sparsely vegetative region, which had decreased vegetation (negative EVI anomalies in Fig. S1) and experienced a negative anomaly in rainfall for much of the year (see Fig. S2), have such large values of carbon uptake? The March – September 2015 posterior carbon uptake values in the sparsely vegetative regions in Figure 6 are larger than any other biome in Australia. Is this not counterintuitive and highly unexpected? Are the larger values due to very large carbon uptake, or is simply due to the large spatial extent of the biome? Could this be due to the choices in prior flux or observational uncertainties which are known to be incorrect (as stated by the authors earlier in the manuscript)? The comparison between CABLE-BIOS3 GPP and MODIS GPP is helpful but does not explain why the carbon uptake in this sparsely vegetative region is so large. This is a very interesting result, but it needs to be explained and interpreted more thoroughly.

In Fig. 9 (in this revision), we plot the prior and the posterior flux estimates not with the same units (PgC y⁻¹) as same the one shown in Fig.6, page 16 in the manuscript. In this case, the carbon fluxes were divided by the area of the ecosystem. It is evident in Fig. 9 that the significant increase in carbon uptake in the sparsely vegetated region of Australia is because a "small shift" in the carbon fluxes over this large ecosystem cause an important impact on the total carbon net flux calculated for the whole country (see Fig. 7). We will include this Figure in the appendix of the main manuscript to show the readers that the big difference seen over sparsely vegetated is mainly because of the large spatial extent of the region.



Figure 9: Monthly time series of the Australian land biosphere prior and posterior CO_2 flux and their uncertainties in gC m⁻² y⁻¹ over six bioclimatic regions. The prior and posterior estimates do not include fossil fuel emissions.

13. There are a couple experimental setups that could just as likely lead to these results instead of it actually occurring in nature. The first thing that needs to be expanded on, and potentially investigated more, is the impact of boundary conditions on the inversion. Small errors in the boundary conditions can have large impacts on regional-scale inversion models. This is evident in Figure 7, as very large adjustments in posterior land fluxes had only small impacts on the XCO2 values (typically ≈0.25 ppm) at the TCCON locations. These same results could be simulated if you had 0.25 ppm or more errors in boundary conditions and had too small prior error uncertainties or did not adjust boundary conditions correctly. Can the authors provide evidence this is not the case? Knowing that observational and prior error uncertainties were not set correctly, how can the mean posterior fluxes values, and spatial distributions, be expected to

be accurate enough to make the claims in the results of this study? Also, the authors clearly state that prior uncertainties are too stiff for ocean fluxes, how do we know that inaccuracies in the ocean prior aren't being redistributed to posterior land fluxes? All three of these concerns could easily lead to similar results/conclusions presented in this study.

This question related to boundary conditions (BCs) was answered in question 2. To avoid the impact of BCs over our optimized fluxes, we extended our CMAQ domain farther away from Australia (see Fig .2). Again, the impact of the BCs was tested in Villalobos et al. (2020). In this study, we showed that the our system is able to reduce the potential biases that BCs might introduce in our inverse system. The question related to uncertainties in the inversion set-up are also answered in question 2.

14. Could this study have assimilated in situ data to infer CO₂ fluxes in Australia? It would be interesting, and perhaps provide more confidence in the results presented here, to see if in situ data assimilation results in similar conclusions compared to inverse model estimates using OCO-2 XCO2 data. Are there any other sources of in situ measurement data in Australia besides the data applied in this study for model evaluation?

We agree with the reviewer that performing a regional inversion with in-situ measurement would have been ideal for quantifying the Australian carbon fluxes with more confidence. But unfortunately, there are not many other sources of in situ measurements in Australia besides the ones applied in this study. For this reason, we only perform a regional inversion using OCO-2 data. If the reviewer wants to know more about Australia monitoring CO_2 site, Ziehn et al. (2014) performed a study over Australia which proposed expanding the current monitoring CO_2 stations over the country. In this work, the authors mention that the current monitoring sites (around six across Australia, which are not all operational) provide no meaningful constraint on Australian fluxes.

15. Have the authors conducted the inversion using OCO-2 XCO2 data for other years than 2015? It would be interesting to see if the model results had any inter-annual variation. Was 2015 selected simply to see if the El Nino had impact on Australia carbon fluxes? If 2015 was in fact an anomalous year, it would be interesting to see if the model framework would not simulate the larger biospheric uptake for later years (e.g., 2017). This could help increase the robustness of the conclusions of this study.

We ran a regional inversion for Australia for 2015-2019 using OCO-2 data (version 9) to assess the inter-annual variability of the Australian CO₂ surface fluxes. These five years inversion is a working paper that focuses on understanding the main climate drivers that may cause inter-annual variability and/or temporal trends in carbon fluxes over Australia. One of the questions in this new article is to evaluate whether the Australian semi-arid ecosystems followed the same patterns observed during 2015 or whether such patterns became stronger or weaker due to precipitation and temperature changes throughout 2015–2019. Australia is a very interesting study case because despite being affected by ENSO in 2015, not all months in 2015 had a deficit of rain, which certainly impacted the net carbon fluxes across Australia (see again Fig.7).



2 Additional analysis: Posterior fluxes derived from OCO-2 MIP

Figure 10: TM5 posterior fluxes using assimilated data from OCO-2 observations (land nadir and land glint data for 2015).

135°E TM5-4DVAR Model

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Land fluxes assimilated by OCO-2 (Land nadir and land glint data) (gC $m^{-2}\;y^{-1})$

40°5

1000

135°E

2000

40°5

-1000

40°5

-2000



Figure 11: CAMS posterior fluxes using assimilated data from OCO-2 observations (land nadir and land glint data for 2015).



Figure 12: PCTM posterior fluxes using assimilated data from OCO-2 observations (land nadir and land glint data for 2015).



Figure 13: CSU posterior fluxes using assimilated data from OCO-2 observations (land nadir and land glint data for 2015).



Figure 14: LoFI posterior fluxes using assimilated data from OCO-2 observations (land nadir and land glint data for 2015).



Figure 15: AMES posterior fluxes using assimilated data from OCO-2 observations (land nadir and land glint data for 2015).



Figure 16: UO posterior fluxes using assimilated data from OCO-2 observations (land nadir and land glint data for 2015).



Figure 17: UT posterior fluxes using assimilated data from OCO-2 observations (land nadir and land glint data for 2015).

Figure 18: CT posterior fluxes using assimilated data from OCO-2 observations (land nadir and land glint data for 2015).

Figure 19: CMS-Flux posterior fluxes using assimilated data from OCO-2 observations (land nadir and land glint data for 2015).

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