

Interactive comment on “The impact of improved satellite retrievals on estimates of biospheric carbon balance” by S. M. Miller and A. M. Michalak

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We thank the referees for their comments and suggestions on the manuscript. Below, we have included the referee’s point-by-point suggestions and the associated changes we have made to the manuscript.

- “Throughout the text, the authors use the expression “robust constraint”, but what is it? If for instance all OCO-2 L4 products had no better quality than the latest biosphere models at any scale, it could be found useless for land vegetation carbon accounting and therefore not robust for that application. I do not think that the chosen method can conclude to robustness. The authors need to qualify their conclusion better: they demonstrate improvement in the retrievals on the basis of

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a specific indicator, but what does this mean in practice?”

We have removed the word “robust” throughout the text when it is used to refer to the flux constraint. The methods section of the article describes, in detail, how the experiments are set up and what they do and do not indicate about the CO₂ flux constraint. Elsewhere in the article, we often use shorter, more concise language to refer to these experiments. Where possible, we have tried to use more specific wording throughout the entire article. Specifically, we have replaced the word “robust” in the following instances throughout the text:

Pg. 2, line 22: replaced with “reliability or accuracy”

Pg. 2, line 23: deleted “and robustness”

Pg. 2, line 25: replaced “robustness” with “detectability”

Pg. 2, line 26: replaced “can be used to robustly constrain fluxes across” with “can be used to identify variations in biospheric fluxes within”

Pg. 2, line 27: deleted “robustly”

Pg. 3, line 10: We have removed this sentence in response to another review comment.

Pg. 5, line 6: replaced “robustness” with “strength”

Pg. 5, line 12: replaced “robustly constrain” with “detect and constrain variations in”

Pg. 5, line 15: replaced “provide a robust constraint” with “can be used to detect variations in”

Pg. 5, line 24: replaced “robustly constraint monthly biospheric fluxes” with “detect spatiotemporal variations in biospheric fluxes”

Pg. 6, line 11: deleted “or robustness”

Pg. 6, line 15: We have edited this sentence in response to another reviewer suggestion.

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Pg. 7, line 18: replaced “as these observations rarely yield a robust constraint for smaller regions” with “as these observations can rarely be used to detect or constrain variations in CO₂ fluxes across smaller regions”.

Fig. 3 caption: replaced “more robust” with “stronger”

- “Crowell et al. (2017) should be updated to Crowell et al. (2019, <http://dx.doi.org/10.5194/acp-2019-87>)”

We have updated this reference in the revised manuscript.

- “P. 3, l.9: the authors actually do not use more than 7 biome regions and therefore do not necessarily reach the point when they are no longer able to detect any variations in biospheric CO₂ sources and sinks.”

We have clarified the text here. We use very large regions in the first two sets of experiments and then shrink those regions down to biome-sized regions in the final set of experiments. This final set of experiments is both a challenging test of current observations and would be an ambitious, ecologically-relevant goal for future inverse modeling studies.

- “P. 3, l. 19: the choice of a year with a strong El Nino episode is surprising. How would the results change with a “normal” year?”

We began working on the preceding companion paper in 2016, and at that time, there was only a single year of OCO-2 observations available to analyze. Hence, both that paper and the current manuscript focus on OCO-2 observations from 2015. In the current manuscript, we have examined the same time period as in the preceding companion paper – to ensure that we can make an apples-to-apples comparison between the two studies. We suspect that results for 2016 would be similar to the analysis for 2015. Environmental conditions in some regions were different in 2015 relative to 2016 due to El Nino, but those differing conditions should not interfere with the regression analysis used in this study;

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many of the predictor variables used in the analysis would differ in 2015 and 2016 to reflect these differing environmental conditions (e.g., EVI, NDVI, and SIF).

- “P. 3, l. 32: the authors need to give details about the seven models so that the reader can get convinced about their realism. For instance, I understand that Miller et al. (2018) used climatological model averages for technical reasons (lack of model availability for the target year): now that model outputs for 2015 are widely available, has this issue been sorted out?”

We have added an SI to the manuscript that describes each of these seven models. This information is also described in the preceding companion paper, and the information in this SI is a duplicate of the information in the preceding companion paper.

Model outputs for 2015 were not available at the time that we began work on the preceding companion paper, and we want to compare apples-to-apples with that paper. There are now biospheric model outputs available for 2015. However, we require a relatively large number of flux model estimates for the statistical model, and there are not a sufficient number of biospheric model outputs that are readily available at a 3-hourly time resolution for 2015. The creation of a new flux model inter-comparison was beyond the scope of the current project. With that said, we have incorporated numerous vegetation indices for 2015 within the statistical model, including SIF, EVI, and NDVI.

- “P. 6, l. 14: I have not seen that the community has deployed significant effort to improve their transport models or their error models in the past years. In comparison, the effort on retrievals, in particular in the OCO-2 team, has been huge. It is not fair to compare them to the rest.”

We have clarified this statement in the revised version of the manuscript, and we have deleted the phrase about retrieval improvements being more attainable than improvements in transport modeling. Our intent here is not to compare improve-

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ments in the retrievals against improvements in meteorology or in biospheric flux modeling. Rather, we wanted to point out that the retrievals, while important, are one factor among many that affect the CO₂ flux constraint.

- “Legends of Figs. 3 and 4: what are target mode retrievals doing here?”

We did not see any reason to exclude target mode observations from the analysis. For example, O’Dell et al. (2018) describe the version 8 ACOS retrieval, and they do not present any evidence to indicate anomalous errors or biases in the target mode observations. We also included target mode observations in the analysis in the preceding companion manuscript, and we want to compare apples-to-apples with the results of that study. The objective of the present manuscript is to compare how the flux constraint has improved as the retrievals have evolved from version 7 to versions 8 and 9. We feel it would be difficult to make that comparison if we used a different approach to analyze versions 8 and 9 than we used to analyze version 7 in the preceding manuscript.

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We thank the referees for their comments and suggestions on the manuscript. Below, we have included the referee’s point-by-point suggestions and the associated changes we have made to the manuscript.

- “It is interesting that the retrieval bias reductions from Version 7 to 8 helped so much with the biospheric flux constraint at the biome-scale. It would be nice for the authors to comment a little more on subtle differences between versions 8 and 9. Looks like the constraint went down in some regions, e.g. the drylands and dry monsoon areas. Why is that?”

We have added text to the revised manuscript to clarify these differences. These

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small differences are due to the stochastic nature of the statistical model. The regression model used in this manuscript requires an estimate of error variances and estimates of the error correlation length and correlation time. We estimate these variances and covariances using a randomized sub-selection of the observations, described in the preceding companion paper; there are too many OCO-2 observations over a year to use all of the observations in that estimation process. Hence, the results of the regression analysis exhibit a small amount of stochasticity depending upon precisely which observations were randomly selected for the variance and covariance estimation. For example, for the simulations shown in the manuscript, we obtained a slightly higher error variance for version 9 ($(0.90 \text{ ppm})^2$) than version 8 ($(0.87)^2 \text{ ppm}^2$) and a slightly longer decorrelation length. This resulted in model selection results for version 9 in which slightly fewer months were selected relative to version 8. We subsequently reran the analysis and then obtained a slightly lower error variance for version 9 relative to version 8 ($(0.83 \text{ ppm})^2$ versus $(0.87)^2 \text{ ppm}^2$). This resulted in model selection results for version 9 in which slightly more months were selected relative to version 8. We have added a brief description of this point in the revised manuscript.

- “Did you try estimating any sub-biome scale regions? Given that the biomes tend to be multi-continental, it would be interesting to see the results using smaller regions that are (mostly) spatially contiguous within a given continent, especially with Versions 8–9.”

It could be interesting to examine sub-biome scale regions. However, the overall motivation of this study was to compare apples-to-apples with the preceding companion paper. In that study, we did not examine smaller regions because we had limited success in constraining fluxes across biome-sized regions. In the present manuscript, by contrast, we were able to detect spatiotemporal variations in CO_2 fluxes within many of these biome-sized regions, a large improvement over re-

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sults using version 7 of the observations.

- “The statement on p. 3, lines 8-10 sounds somewhat misleading: ‘We begin with large, hemispheric regions and then decrease the size of those regions until we are no longer able to detect any variations in biospheric CO₂ sources and sinks.’ It looks like you could potentially go to even finer spatial scales in the tropical grasslands/ forests and drylands/ dry monsoon biomes with Version 8 9 retrievals.”

The reviewer raises a good point, and reviewer #1 made a similar suggestion. We have revised this statement in the manuscript accordingly.

- “This may not be the focus of your study, but I was very curious to see the results of your model selection and estimated betas from the regression with the selected bio models (and anthro/ biomass burning/ ocean fluxes). Which biospheric models were selected in different region/ month combinations? When was just one model selected vs. multiple models? Can these results help to inform which models are performing best in which regions? Does the ‘best’ model for a given month change as a function of spatial scale? This could be potentially useful information for biospheric model developers. Also, I don’t see a supplemental material, but do you list anywhere which bio models went into the model selection algorithm?”

We agree; model selection can be a useful tool to help identify patterns in CO₂ fluxes that are or are not consistent with atmospheric observations. A number of studies have used model selection to explore which flux patterns and which biosphere models are best able to reproduce atmospheric observations. For example, Fang et al. (2014) and Fang and Michalak (2015) explore these questions using in situ CO₂ observations. We agree that these are interesting questions but feel that these questions are beyond the scope of the current study and would be better answered in a separate future, study. Adding that analysis to the present

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study would arguably complicate or distract from the framing and messaging of the current manuscript.

- “Not clear why you would include or exclude glint observations. It looks like in Miller et al, 2018, you exclude glint observations from results shown in the main manuscript. Why? How has the quality of these observations improved in Versions 8 and 9? And why are glint observations helping especially in tropical regions? Are they able to improve the density of observations in cloud-covered areas, or is a single glint measurement more informative than a single nadir or target measurement in these regions? Please don’t assume too much satellite-based knowledge on the part of the reader!”

The reviewer makes a really good point about not assuming too much satellite-based knowledge on the part of the reader. We have added more explanation on this topic in the revised manuscript. In brief, glint observations have historically had much higher error variances and larger biases relative to nadir observations. For example, land glint observations in version 7 had a ~0.5ppm offset compared to land nadir observations (e.g., O’Dell et al. 2018). Until recently, it was arguably very challenging to include both types of observations in an inverse model because one type had a fundamentally different magnitude relative to the other. In the preceding companion paper (Miller et al. 2018), we included results using glint observations within the SI, but we did not put great emphasis on these results with glint observations because of their known biases.

By contrast, the accuracy of the glint observations greatly improved markedly with version 8 of the observations. In fact, the largest improvements between versions 7 and 8 of the observations was to the glint observations, and these improvements greatly reduced the bias between land nadir and land glint observations (O’Dell et al. 2018). These improvements arguably make it feasible to assimilate land nadir and land glint observations in the same top-down framework or inverse model.

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We have also included more explanation in the revised manuscript about the improvements tropical biomes versus mid- and high-latitude biomes. The results using versions 7 and 8 show the greatest differences across tropical biomes. This feature is most likely because there is a large signal-to-noise ratio in many tropical biomes throughout the year, whereas the signal-to-noise ratio in mid- and high-latitudes is only large during northern hemisphere summer. Phrased differently, there is a consistent flux signal from many tropical regions throughout the year, and hence we are able to detect variations in fluxes from tropical regions across different seasons using version 8 of the observations. By contrast, net ecosystem exchange (NEE) in northern mid- and high-latitudes has the largest absolute magnitude during northern hemisphere summer. As a result, we see a large improvement in the flux constraint in mid-latitudes in northern hemisphere summer but not in other times of year when the absolute magnitude of NEE is smaller. Furthermore, there are far fewer land nadir and land glint observations in northern mid- and high-latitudes in northern hemisphere winter.

- “* P. 3, lines 31-33: it might be nice to put an equation or diagram or even table here showing the potential inputs that go into the model selection and your regressions. Do you run model selection on all months simultaneously? That’s what it sounds like, but please make that more clear.”

We have added text to the revised manuscript to clarify. We do run all months simultaneously. We have also added an equation to the manuscript to summarize the regression:

$$z = h(\mathbf{X})\beta + b + \epsilon$$

where z are the OCO-2 observations, \mathbf{X} the different predictor variables, $h()$ an atmospheric transport model (in this case PCTM), β the coefficients estimated in the regression, b the model spinup or CO₂ mixing ratios at the beginning of the experiments, and ϵ the model–data residuals. Note that there are different columns of \mathbf{X} corresponding to each biospheric flux model in each different month and

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each different biome. Model selection will determine which columns of \mathbf{X} can best reproduce the OCO-2 observations without overfitting those observations.

This equation and the associated explanation is also included in the preceding companion paper.

- “* P. 4, lines 4 and 8: please replace the terms ‘former’ and ‘latter’ with something more descriptive, e.g. biospheric model output and constant fluxes.”

We have edited the text accordingly. We have replaced the word “former” with “some of the model outputs that use a flux model or vegetation index,” and we have removed the word “latter.”

- “* P. 4, line 19: ‘to avoid potentially biasing the results’. This is true, but please make clear that XCO₂ reflects the contributions of all these different types of fluxes (ocean/ FF/ BB/ terrestrial bio), so you need to account for the non-bio fluxes in order to isolate the signal of the bio in the regression. Can also comment that the uncertainty on the FF/ ocean/ BB fluxes is thought to be much smaller than that on the terrestrial bio fluxes (with reference).”

The reviewer makes a great point, and we have edited the text accordingly.

We have also added text to the manuscript explaining that biospheric fluxes are thought to be more uncertain than other CO₂ source types. For example, we have cited the National Academy of Science Report on fossil fuel CO₂ emissions (NAS 2010) and have cited a biosphere flux model intercomparison paper (Huntzinger et al. 2012) and a Global Carbon Project assessment (Le Quéré et al. 2018) as evidence of these differing uncertainties.

- “* P. 5, line 13: ‘in about half of all months in the tropics’, but didn’t you say on line 10 that ‘variations in CO₂ fluxes are detectable across tropical biomes much of the year?’ In Version 9, it looks like you can constrain bio fluxes in the tropical grasslands and forests for 8 and 9 months of the year, respectively”

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The reviewer is correct – the number cited in the manuscript should be two thirds, not one half. That is an error on our part. We have updated the text accordingly.

- “P. 6, line 17: please add references for the ACOS retrievals and bias correction, and also for OCO-3 and GeoCarb.”

We have added references to this line accordingly. We have added citations to O'Dell et al. (2012) and O'Dell et al. (2018) for the ACOS retrieval, Eldering et al. (2019) for OCO-3, and Polonsky et al. (2014) for GEOCarb.

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The impact of improved satellite retrievals on estimates of biospheric carbon balance

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Abstract. The Orbiting Carbon Observatory 2 (OCO-2) is NASA's first satellite dedicated to monitoring CO₂ from space and could provide novel insight into CO₂ fluxes across the globe. However, one continuing challenge is the development of a robust retrieval algorithm: an estimate of atmospheric CO₂ from satellite observations of near infrared radiation. The OCO-2 retrievals have undergone multiple updates since the satellite's launch, and the retrieval algorithm is now on its ninth version. Some of these retrieval updates, particularly version 8, led to marked changes in the CO₂ observations, changes of 0.5 ppm or more. In this study, we evaluate the extent to which current OCO-2 observations can constrain monthly CO₂ sources and sinks from the biosphere, and we particularly focus on how this constraint has evolved with improvements to the OCO-2 retrieval algorithm. We find that improvements in the CO₂ retrieval are having a potentially transformative effect on satellite-based estimates of the global biospheric carbon balance. The version 7 OCO-2 retrievals formed the basis of early inverse modeling studies using OCO-2 data; these observations are best-equipped to constrain the biospheric carbon balance across only continental or hemispheric regions. By contrast, newer versions of the retrieval algorithm yield a far more detailed constraint, and we are able to constrain CO₂ budgets for seven global biome-based regions, particularly during the Northern Hemisphere summer when biospheric CO₂ uptake is greatest. Improvements to the OCO-2 observations have had the largest impact on glint mode observations, and we also find the largest improvements in the terrestrial CO₂ flux constraint when we include both nadir and glint data.

1 Introduction

Over the past five years, the field of CO₂ remote sensing has evolved rapidly. The sheer number of satellites has increased with the launch of TanSat in 2016 (Yang et al., 2018), GOSAT-2 in 2018 (e.g., Nakajima et al., 2012), and OCO-3 in 2019 (e.g., Eldering et al., 2019). Several additional satellites have also been funded or proposed (e.g., Polonsky et al., 2014; Tollefson, 2016). In addition, the actual CO₂ observations or satellite retrievals have also been changing. Roughly once per year, the NASA Atmospheric CO₂ Observations from Space (ACOS) science team releases a new version of the OCO-2 and GOSAT observations that incorporates the most recent advances in the retrieval algorithm and addresses observational errors that have been identified by the scientific community (e.g., O'Dell et al., 2012). Early top-down studies of CO₂ fluxes using OCO-2 employed version 7

of the observations (~~e.g., Chatterjee et al., 2017; ?; Liu et al., 2017; Nassar et al., 2017~~)(e.g., Chatterjee et al., 2017; Crowell et al., 2019; Liu et al., 2017; Nassar et al., 2017), but the ACOS team has subsequently updated the observations through version 9 (at the time of writing).

The OCO-2 observations have changed markedly through this process. One of the largest changes occurred with the release of version 8 of the OCO-2 observations in September 2017 (Fig. 1). This update incorporated a multitude of changes to the quality control prescreening process, the forward spectroscopy model, the retrieval algorithm, and the bias correction (O'Dell et al., 2018b). These changes led to widespread improvements in the observations; version 8 has smaller random errors when compared to ground-based observations, a smaller bias between land nadir and land glint observations, and less bias across many northern high-latitude terrestrial regions (Wunch et al., 2017; O'Dell et al., 2018b). ~~Several specific improvements are particularly notable~~These improvements had a particularly large impact on glint mode observations. For example, a correction to the averaging kernel reduced a 0.3ppm bias in land glint data relative to land nadir (O'Dell et al., 2018b). Previously, inverse modeling studies using version 7 of the OCO-2 retrieval did not assimilate land glint and land nadir observations simultaneously due to this bias (e.g., Crowell et al., 2019). Furthermore, version 7 glint observations had biases greater than 1ppm across the southern ocean that have been remedied in version 8. These errors appeared to be due to high altitude aerosols, so the version 8 algorithm includes a new aerosol layer in the upper troposphere and lower stratosphere that has remedied many of these biases. Furthermore, a correction to the averaging kernel reduced the 0.3ppm bias between land nadir and land glint data (O'Dell et al., 2018b). Overall, the observations rated as good quality in version 8 are very different from those in version 7; 24% of the observations that were marked as high quality in version 7 have been marked as low quality in version 8, and 34% of the observations marked as high quality in version 8 were marked as low quality in version 7.

More recently, version 9 of the OCO-2 observations has been released in October 2018. Improvements in version 9 of the retrieval algorithm yielded smaller changes in the observations (O'Dell et al., 2018a). In particular, this version includes a correction for small-scale biases over land due to topography. Furthermore, the ACOS team relaxed a filter that discards observations collected over dark surfaces, and this change yields more observations over tropical forests (O'Dell et al., 2018a). In spite of these advances, there are still many opportunities for further improving the retrievals. For example, OCO-2 retrievals appear to show biases across most of the northern tropical oceans (O'Dell et al., 2018b).

These improvements to the observations should also improve the ~~robustness-reliability or accuracy~~robustness-reliability or accuracy of CO₂ fluxes estimated using the observations. Several studies indicate that errors in the retrieval can have a substantial impact on ~~strength and robustness-the strength~~strength and robustness-the strength of the CO₂ flux constraint (~~e.g., Chevallier et al., 2007; Baker et al., 2010; ?; Miller et al., 2018~~)(e.g., Chevallier et al., 2007; Baker et al., 2010; Crowell et al., 2019; Miller et al., 2018). For example, Miller et al. (2018) explored the ~~robustness-of-the-detectability of~~robustness-of-the-detectability of biospheric CO₂ ~~flux-constraint fluxes~~flux-constraint fluxes using version 7 of the OCO-2 observations. They found that OCO-2 observations can be used to ~~robustly-constrain fluxes-across-identify variations in biospheric fluxes within~~robustly-constrain fluxes-across-identify variations in biospheric fluxes within continental or hemispheric regions but that the observations have limited ability to ~~robustly-estimate-constrain~~robustly-estimate-constrain biospheric CO₂ fluxes across smaller regions. The authors constructed a series of synthetic data experiments to understand the most important factors ~~driving these results-limiting the CO₂ flux constraint~~driving these results-limiting the CO₂ flux constraint; they concluded that atmospheric transport errors and prior flux errors play a role, but retrieval errors are a particularly salient factor. The OCO-2 science team is also developing an ensemble of inverse modeling estimates of CO₂ fluxes, and recent comparisons show results that are broadly parallel to

Miller et al. (2018): inverse models provide consistent CO₂ flux totals for continents or hemispheres but diverge for smaller regions (e.g., ?)(e.g., Crowell et al., 2019).

The present study is a follow-up to Miller et al. (2018). We re-examine the conclusions of that study in light of recent improvements in OCO-2 observations of CO₂. We also identify opportunities for future improvements to the retrievals.

5 2 Methods

2.1 Overview

~~We~~ Uncertainties in biospheric fluxes are thought to be greater than in other CO₂ source types (e.g., National Research Council, 2010; Hunt , and the CO₂ signal from biospheric fluxes is often larger than from other source types. Hence, we design a set of top-down experiments to examine whether we can detect variations in biospheric CO₂ sources and sinks within different regions of the globe and different months of the year using OCO-2 observations. In the present study, these variations are defined as any spatial or temporal patterns in CO₂ fluxes that have been gridded to the resolution of a global atmospheric model – ~~one degree latitude by one degree~~ 1° latitude by 1.25° longitude and a 3-hourly time interval.

Detecting variations in CO₂ fluxes is a pre-requisite for constraining CO₂ budgets or flux totals; we must be able to detect variations in CO₂ sources and sinks across a region if we are to constrain budgets across any region of smaller size. We begin with ~~large, two large~~ hemispheric regions and then decrease the size of those regions ~~until we are no longer able to detect any variations in biospheric CO₂ sources and sinks to create increasingly challenging tests of the OCO-2 observations~~ (Fig. 2). ~~That limit is the smallest region for which we could robustly estimate CO₂ fluxes using currently available OCO-2 observations; we use four and seven global regions, respectively, in each of these experiments.~~ All of these regions are based on a map of global biomes presented in Olson et al. (2001). The seven-region map contains broad global biomes aggregated from those in Olson et al. (2001) while the two- and four-region maps have been aggregated from Olson et al. (2001) to form even larger regions. We use a biome-based map because inverse modeling studies often estimate CO₂ flux totals for biome-based regions, and these regions have clear ecological significance.

We construct this set of experiments for each of the last three versions of the OCO-2 observations and examine how the results change with the retrieval version. These experiments are identical except for the retrieval version used. Therefore, this setup provides a means to understand how improvements in the observations are improving the constraint on biospheric CO₂ fluxes. We examine these questions for each month within the year 2015 – to understand how these results vary by season and by region or biome.

2.2 Implementation of the top-down experiments

We design a regression framework to determine whether we can detect variations in CO₂ fluxes using OCO-2 observations. This section provides an overview of the approach, but Miller et al. (2018) provides full descriptive and mathematical detail. This regression will try to match CO₂ observations from OCO-2 using numerous atmospheric model outputs. Each model

output estimates the enhancement in total column CO₂ (XCO₂) from fluxes in a particular region and a particular month. We generate all of these model outputs of CO₂ using the Parameterized Chemistry and Transport Model (PCTM) (Kawa et al., 2004). The model setup used here has a spatial resolution of ~~one-degree latitude by one degree~~ 1° latitude by 1.25° longitude, and we incorporate CO₂ fluxes at a 3-hourly time resolution. The wind fields used to drive PCTM are from the Modern Era
5 Retrospective-Analysis for Research and Applications (MERRA) product (Rienecker et al., 2011). This setup is identical to Miller et al. (2018).

We run many atmospheric model simulations using numerous different biospheric CO₂ flux estimates. The regression will try to reproduce OCO-2 observations using a linear combination of these model ~~outputs~~ simulations. For example, in the seven region experiments, we use seven different geographic regions, seven biospheric CO₂ flux estimates, and 16 different months
10 (September 2014-December 2015). We discard results from the first four months as model spin-up. These combinations equate to 784 total atmospheric model outputs. We further run atmospheric model simulations using a spatially and temporally constant flux in each region and each month, and we allow the regression to use these model outputs as well. The SI and Miller et al. (2018) describe the CO₂ flux estimates and regression in greater detail.

This approach provides a means to evaluate when and where current satellite observations can constrain variations in CO₂
15 fluxes. At least some of the ~~former-model-outputs~~ atmospheric model outputs that are driven by biospheric CO₂ flux estimates should help reproduce the OCO-2 observations better than the model outputs that are driven by spatially and temporally constant fluxes. If so, a model with spatially and temporally variable fluxes is better able to reproduce OCO-2 observations than a model with constant fluxes. This result would imply that OCO-2 observations can be used to detect variations in biospheric CO₂ sources and sinks within a given region for a given month. By contrast, suppose that the ~~former-model-outputs~~ atmospheric
20 model outputs driven by biospheric CO₂ flux estimates do not reproduce the OCO-2 observations any better than the ~~latter~~ model outputs with constant CO₂ fluxes. This result would imply one of several conclusions. First, the observations may not be sensitive to fluxes from the region or month in question. This outcome may occur if the magnitude of fluxes is small in a given region or if there are no OCO-2 observations near that region. Second, errors in the atmospheric model or in the OCO-2 observations may obscure variations in XCO₂ that are due to CO₂ fluxes. Lastly, the biospheric CO₂ flux estimates used in the
25 atmospheric model may not be skilled and may not reflect real-world biospheric CO₂ fluxes. However, in this study, we offer up seven biospheric CO₂ flux estimates for each region and each month, and at least one of these estimates should correlate with real-world CO₂ fluxes to a reasonable extent. Hence, it is unlikely that this explanation would drive the results. Rather, it is more likely that the observations are not sensitive to fluxes from a given region or that errors in the model–data system are too large.

Note that ~~we also account for the contribution of non-biospheric fluxes within the regression. Anthropogenic~~ anthropogenic,
30 biomass burning, ~~and ocean fluxes are not the focus of this study. However, we include these fluxes within the regression~~ nonetheless to avoid potentially biasing the results ocean, and biospheric fluxes all contribute to XCO₂ observed by OCO-2,
and we need to account for non-biospheric CO₂ fluxes in order to isolate the signal from biospheric fluxes in the regression.
We model atmospheric enhancements of XCO₂ from anthropogenic emissions using EDGAR v4.2 FT2010 (European Com-
35 mission, Joint Research Centre (JRC)/Netherlands Environmental Assessment Agency (PBL), 2013; Olivier et al., 2014), cli-

matological ocean fluxes using Takahashi et al. (2016), and biomass burning fluxes using the Global Fire Emissions Database (GFED), version 4.1 (van der Werf et al., 2010; Giglio et al., 2013); each of these model outputs is considered in the regression.

We further implement model selection to evaluate when and where current satellite observations can constrain variations in biospheric CO₂ fluxes. Model selection will determine which combination of atmospheric model outputs to include in the regression based upon which best reproduces the OCO-2 observations. If this combination includes at least one biospheric CO₂ flux model for a given region and season, we conclude that the observations likely can be used to constrain variations in CO₂ fluxes. However, if this combination does not include any biospheric CO₂ flux model for a given region and season, we conclude that the observations likely cannot be used to constrain flux variations for that region and season.

We specifically employ a form of model selection known as the Bayesian Information Criterion (BIC), an approach commonly used in regression modeling (e.g., Ramsey and Schafer, 2012, chap. 12) and more recently in atmospheric inverse modeling (e.g., Gourdji et al., 2012; Miller et al., 2013; Shiga et al., 2014; Fang et al., 2014; Fang and Michalak, 2015). To this end, we create different combinations of model outputs and use each combination in the regression. We score each combination based upon how well it reproduces the OCO-2 observations; combinations with a lower weighted sum of squares error receive a better score. Each combination is also scored based upon the total number of model outputs in that combination. Specifically, combinations with a greater number of model outputs receive a larger penalty for complexity, and this penalty prevents combinations that overfit the data from receiving an anomalously good score. The best combination of atmospheric model outputs is the one with the lowest score. We subsequently examine this combination and tally whether at least one atmospheric model output using a biospheric flux estimate was selected for each region and each month of the year. Miller et al. (2018) describes and the SI describe this approach in greater detail, including the specific equations for the BIC.

20 3 Results & discussion

3.1 Robustness Strength of the biospheric CO₂ flux constraint

The constraint on CO₂ fluxes using recent versions of the OCO-2 observations is a step-change improvement relative to previous versions. Overall, there was only a limited ability to detect variations in monthly CO₂ fluxes across individual biomes using version 7 of the retrievals (Miller et al., 2018, Fig. 3a-e) (Fig. 3a-c, Miller et al., 2018). However, these capabilities have changed using versions 8 and 9 of the observations (Fig. 3d-i). Variations in CO₂ fluxes are detectable across tropical biomes much of the year and across temperate biomes in northern hemisphere summer when fluxes from these regions are most variable. These results imply that the updated OCO-2 observations can be used to robustly constrain detect and constrain variations in monthly CO₂ fluxes from seven biome-based regions in certain circumstances – in about half two thirds of all months in the tropics and during northern hemisphere summer in the extra-tropics.

30 The improvement in the flux constraint is particularly evident in the four- and seven-region experiments (Figs. 3b-c and 3e-f). In the four-region model selection experiments, the OCO-2 observations provide a robust constraint on can be used to detect variations in tropical fluxes for most months of the year (Fig. 3e). In other words, at least one biosphere flux model is found to explain a sufficiently large fraction of the observed variability in XCO₂ as to be selected via the BIC model selection

procedure for the tropical regions for most months. This result indicates that spatiotemporal variability in CO₂ fluxes from within each of these regions is preserved in the OCO-2 observations. This represents a marked improvement over results when using observations from version 7 of the OCO-2 retrieval algorithm (Figs. 3b and 3e, Miller et al., 2018). The results using the newer versions 8 and 9 also show substantial improvements in other regions, including dryland and dry monsoon regions, 5 temperate regions, and high-latitude regions (Figs. 3e and 3h).

The seven-region model selection experiments are an even more challenging test of current observations. These experiments examine whether we can ~~robustly constraint monthly~~ detect spatiotemporal variations in biospheric fluxes across seven broad, aggregated global biomes. These experiments produce much better results using versions 8 and 9 of the observations. Specifically, biospheric flux models are selected across tropical and subtropical biomes for at least one month of every season. The 10 same is true across all temperate and high-latitude biomes for a minimum of one month during northern hemisphere summer.

These improvements appear greatest across tropical biomes. There is a consistent flux signal from many tropical regions throughout the year, and hence we are able to detect variations in fluxes from tropical regions across different seasons using versions 8 and 9 of the observations. By contrast, the atmospheric signal due to biospheric CO₂ fluxes in northern mid- and high-latitudes has the largest absolute magnitude during northern hemisphere summer. As a result, we see a large improvement 15 in the flux constraint in mid-latitudes in northern hemisphere summer but not in other times of year when the absolute magnitude of CO₂ fluxes is smaller. Furthermore, there are far fewer land nadir and land glint observations in northern mid- and high-latitudes in northern hemisphere winter relative to summer.

One notable feature of all model selection experiments is the result for dryland and dry monsoon regions (Fig. 2c). At first glance, it may appear surprising that biospheric flux models are selected for so many months in this region, given that some 20 parts of this region are very dry and presumably have small CO₂ fluxes. Several semiarid regions within this classification have a very distinct monsoon that can bring over 500mm of precipitation per month (e.g., northeastern Brazil, western India, and Pakistan). As a result, there is a large spatial contrast in CO₂ fluxes across these regions during northern hemisphere spring and summer – large CO₂ uptake in places with a spring and summer monsoon and little to no fluxes in places like the Sahara or the Arabian Peninsula.

25 Note that the results using version 9 of the observations are not very different from those using version 8. The change in the observations between versions 8 and 9 is only incremental (e.g., Fig. 1b). Version 9 has a lower quality control threshold for surfaces with low albedo, resulting in more observations across tropical rainforests (O'Dell et al., 2018a), and this version includes a topography correction that mostly manifests at small spatial scales. The latter change could be very important for studies that estimate point sources or urban emissions using OCO-2. However, these changes are unlikely to make a large 30 difference in this study both given the large size of the regions examined and the 1° × 1° spatial resolution of the atmospheric model simulations. The SI includes a detailed discussion of the subtle differences between the model selection results using versions 8 and 9 of the observations.

3.2 Drivers of the results

Numerous factors affect the accuracy ~~or robustness~~ of CO₂ fluxes estimated from satellite data. These factors include the accuracy and precision of the observations, the atmospheric transport model, and the prior flux estimate used in the inverse model. ~~Arguably, improvements~~ Improvements in any of these inverse modeling inputs could improve the constraint on biospheric CO₂ fluxes. ~~However, improvements in the observations have arguably been more attainable than these other factors, and we find that these improvements~~ We find that recent improvements to the retrieval are having a particularly large impact on the ~~robustness~~ strength of the CO₂ flux constraint. Furthermore, these improvements are not restricted to a single satellite like OCO-2. Rather, the ACOS retrievals and bias correction (O'Dell et al., 2012, 2018b) will be directly applicable to other NASA carbon monitoring missions, including the recently-launched OCO-3 mission (Eldering et al., 2019) and the planned GeoCarb mission (Polonsky et al., 2014).

These improvements to the retrieval algorithm have had an effect on both glint and nadir observations from OCO-2 collected in almost every region of the globe. The sheer number of different changes makes it challenging to pinpoint exactly which have had the largest impact on the CO₂ flux constraint; there have been numerous updates to the quality control prescreening, the forward spectroscopy model, the retrieval algorithm, and the bias correction. Furthermore, these updates have had multiple effects on the reported CO₂ observations, reducing white noise, reducing bias, and changing which observations do or do not pass quality control. O'Dell et al. (2018b) detail these changes in much greater detail.

With that said, a few of these improvements appear to have a particularly salient impact on the results of this study. For example, the largest improvements have generally been to the glint mode observations. A 0.2 to 0.3 ppm bias between land nadir and land glint observations in version 7 has been remedied in version 8, and version 8 glint observations show smaller biases across many ocean regions. Furthermore, version 8 exhibits less random noise in all types of observations, but that noise reduction is largest in glint observations, both over land and over the oceans (O'Dell et al., 2018b).

Indeed, we also see the largest improvement in the flux experiments conducted in this study when we include glint mode observations. Figure 4 displays the results of the model selection experiments when the glint data are excluded. The figure shows results using version 7, and 8, and 9 of the observations. The improvement between versions 7 and 8 is much smaller when the glint observations are excluded than when they are included (Fig. 3). Even in terrestrial regions, these glint observations may play a key role in the overall flux constraint. For example, the absolute number of nadir and glint observations over land are roughly equal; there are 4.3×10^6 land nadir observations with a positive quality control flag for 2015 and 4.3×10^6 land glint observations during the same time period.

Note that this study focuses on detecting variations in CO₂ fluxes from terrestrial regions in individual months. To that end, certain types of flux estimation problems are beyond the scope of the current study. For example, there is strong evidence that OCO-2 observations are still biased across northern tropical oceans, and reductions in these biases could improve ocean flux estimates derived from OCO-2 (Baker, 2018; O'Dell et al., 2018b). Furthermore, there is always a possibility that the observations have a bias that is correlated across regions larger than those examined in this study. For example, the observations

show a small, time-dependent drift from one year to another (O'Dell et al., 2018b). The approach used in this study would be unlikely to detect the impact of those biases.

4 Conclusions

CO₂ observations from the OCO-2 satellite have changed enormously with recent improvements to the retrieval algorithm. New observations are more self-consistent (e.g., better agreement between glint and nadir data) and compare better against ground-based observations. In some regions, these changes are comparable in magnitude to the atmospheric CO₂ enhancement due to biospheric CO₂ sources and sinks.

In this study, we specifically examine how these changes to the retrieval algorithm have improved the constraint on biospheric CO₂ fluxes, and we find that the improvement is large. Using observations based on version 7 of the retrieval algorithm, we find that biospheric fluxes can only be constrained across continental or hemisphere-size regions, as these observations ~~rarely yield a robust constraint for~~ can rarely be used to detect or constrain variations in CO₂ fluxes across smaller regions. By contrast, we find a step-change improvement in the biospheric CO₂ flux constraint using updated versions of the OCO-2 observations, based on versions 8 and 9 of the retrieval algorithm. Specifically, these improvements make it possible to ~~robustly constrain detect~~ variations in CO₂ fluxes ~~across~~ within seven global biome-based regions during many seasons of the year. This improvement is particularly large when both nadir and glint data are included.

This study indicates that improvements to space-based CO₂ observations are yielding large improvements in global monitoring of biospheric carbon fluxes. As new CO₂ monitoring missions like OCO-3 and GeoCarb launch into orbit, these improvements will have a lasting impact on space-based monitoring of CO₂.

Data availability. All OCO-2 observations are available from NASA's Goddard Earth Sciences Data and Information Services Center (GES DISC) at <https://disc.gsfc.nasa.gov/OCO-2> (last access: 24 Feb. 2019).

Author contributions. S.M.M and A.M.M. designed and wrote the study.

Competing interests. The authors declare that they have no conflicts of interest.

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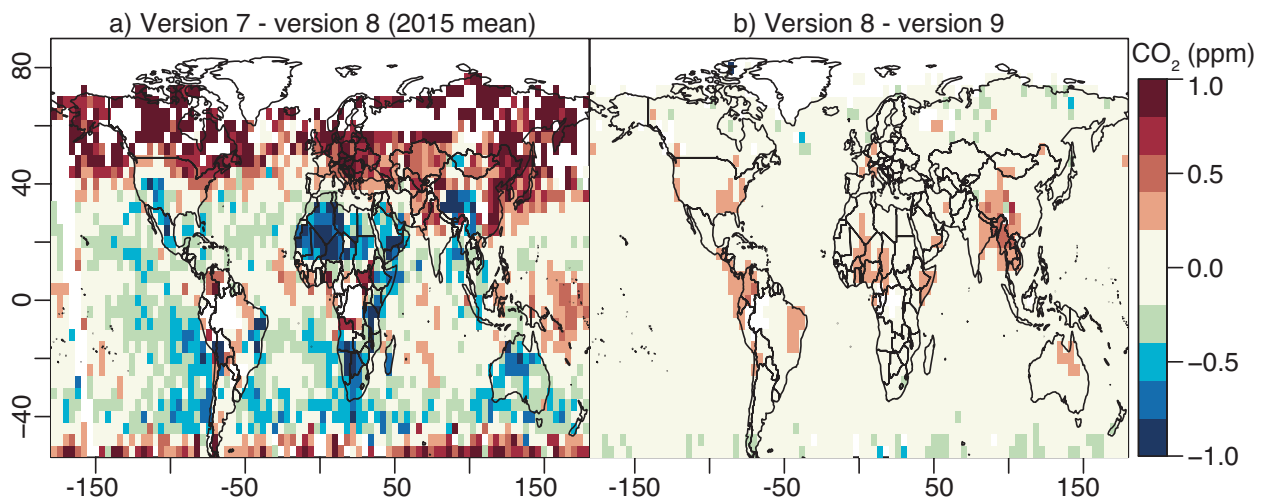


Figure 1. Differences between versions 7 and 8 of the OCO-2 observations (a) and between versions 8 and 9 of the observations (b). Version 8 was a much larger update to the observations than version 9. We average all of the differences between observations onto a grid to make the differences more visually apparent. The results shown here are for observations collected in 2015, the time period analyzed in this study. In addition, this map only displays grid boxes with more than 250 total observations in 2015.

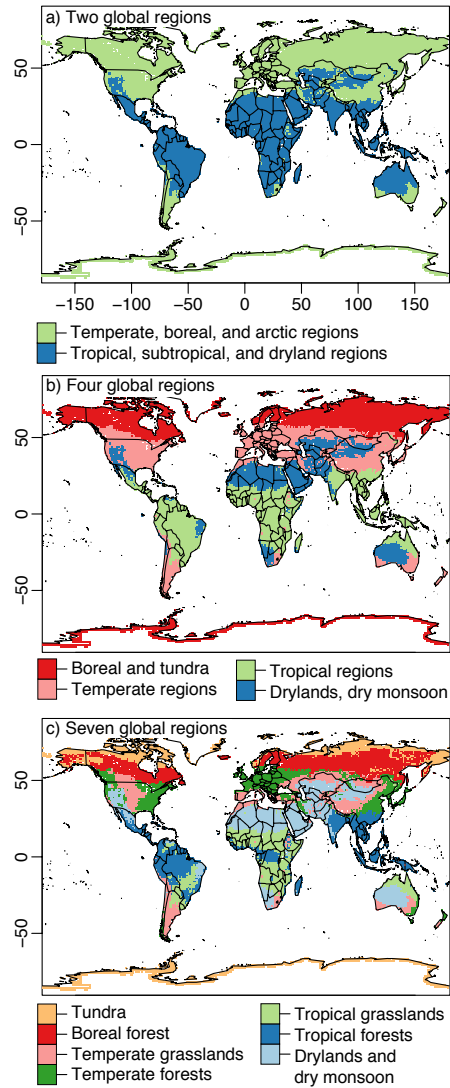


Figure 2. The two hemispheric regions (a), four continental regions (b), and seven biome-based regions (c) used in this study. These regions are based upon the world biome map by Olson et al. (2001). The two- and four-region maps are constructed by aggregating individual biomes into larger regions.

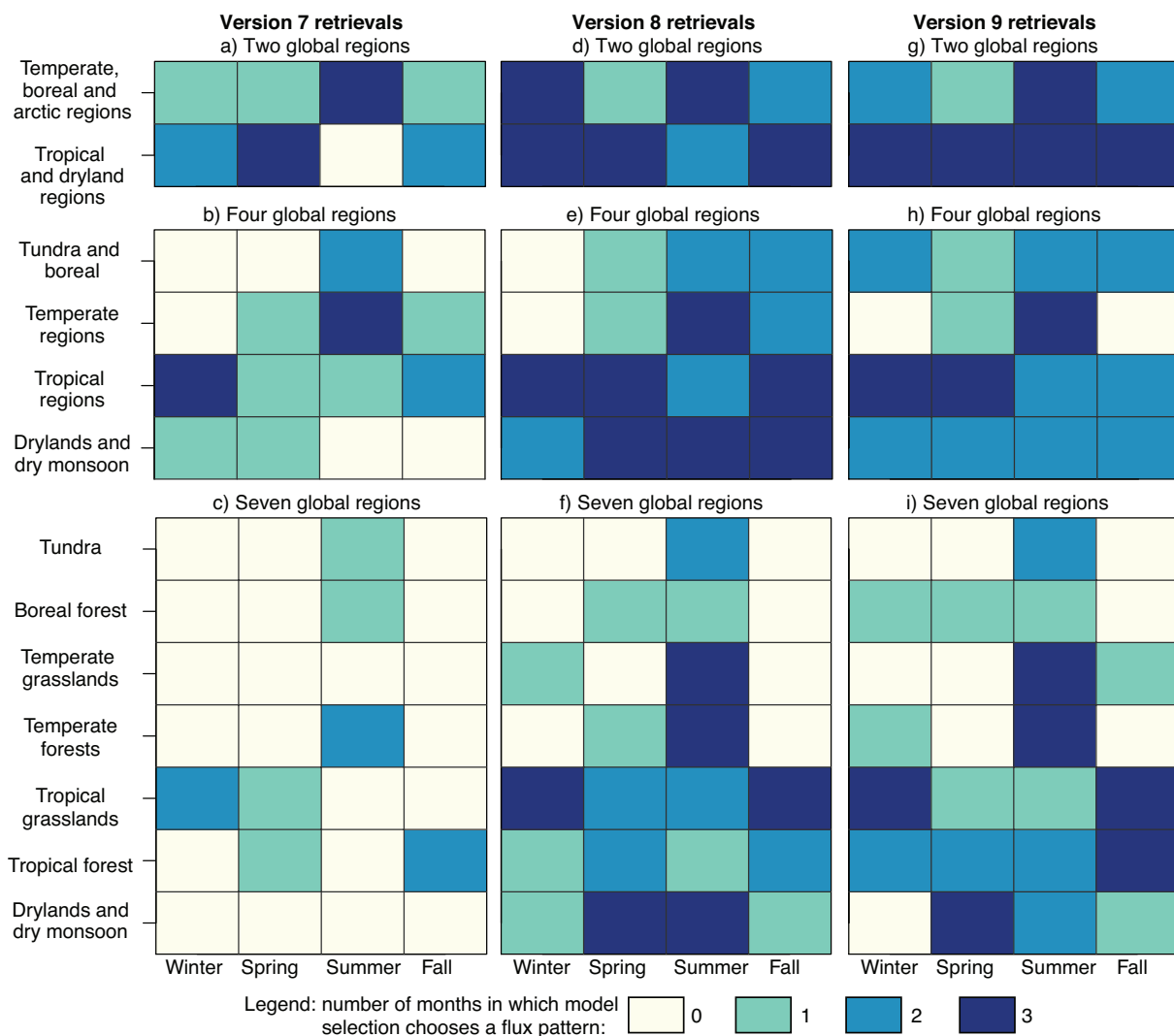


Figure 3. Results of the model selection experiments using versions 7, 8, and 9 of the OCO-2 observations. Versions 8 and 9 provide a much **more-robust-stronger** constraint on biospheric CO₂ fluxes than version 7. The top row displays the results of the experiments with two global regions, the second row with four global regions, and the third row with seven global regions. Each box is color-coded based upon the number of months in which at least one biospheric flux model is chosen using model selection. Dark colors indicate a **robust-strong** constraint on monthly CO₂ fluxes while light colors indicate a weak constraint. Note that these experiments include nadir, target, glint mode observations. In addition, version 7 results are the same as those in Miller et al. (2018).

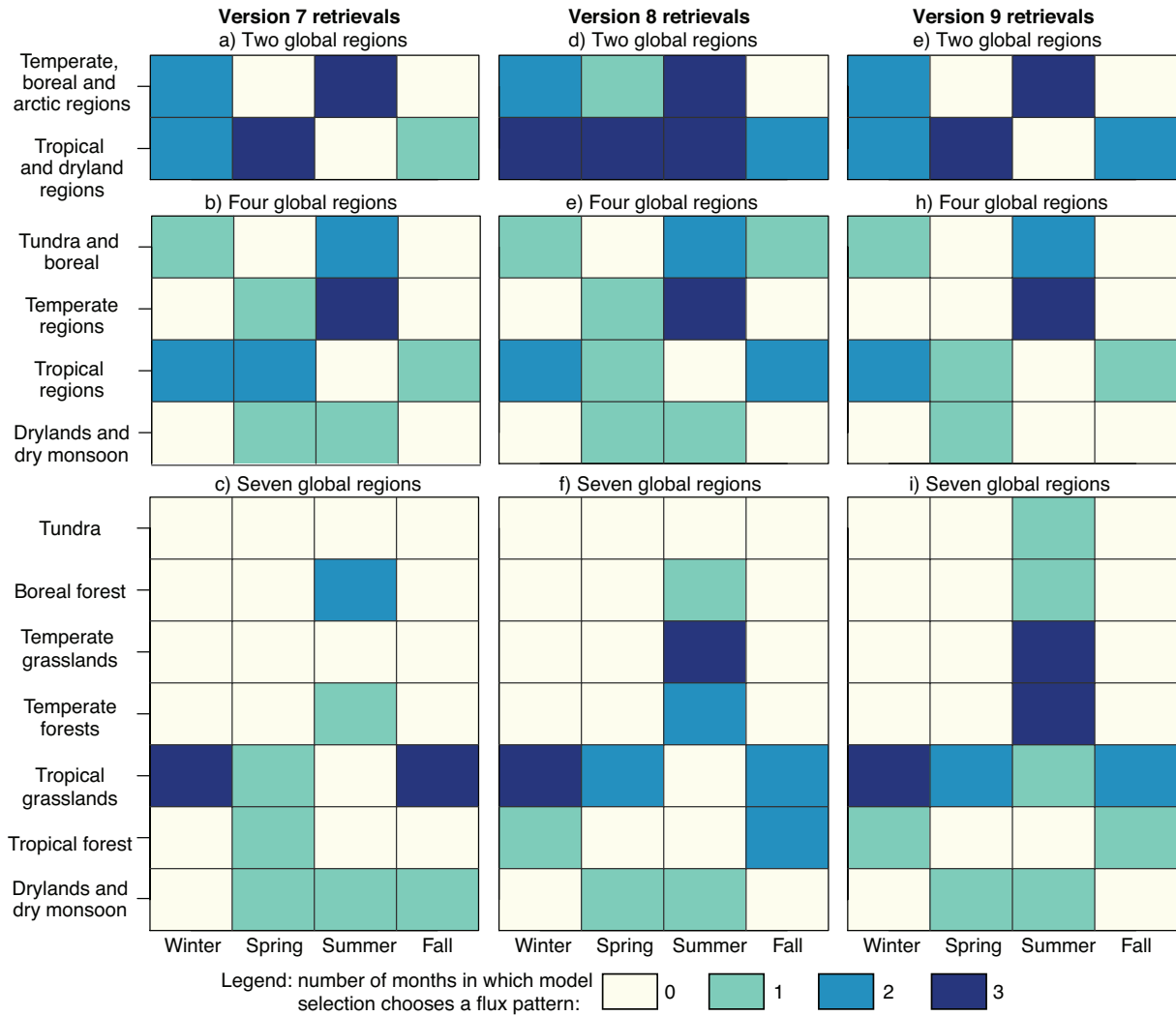


Figure 4. Results of the model selection experiments using only nadir and target mode observations. The improvement between versions 7 and 8 is less pronounced when we exclude glint observations and include only nadir and target mode data. Version 7 results here are the same as those in Miller et al. (2018).

S1 The regression and model selection framework

We construct a series of statistical experiments to evaluate whether we can detect spatial and temporal variations in biospheric CO₂ fluxes within different global regions using current OCO-2 observations. This section of the SI describes these experiments in greater detail. This approach is identical to Miller et al. (2018), and that study provides additional detail.

These experiments are based upon a regression framework, as described in the main article. The regression has the following form:

$$\underline{z} = \underline{h(\mathbf{X})}\beta + \underline{\mathbf{b}} + \underline{\epsilon} \quad (\text{S1})$$

where \underline{z} (dimensions $n \times 1$) are the OCO-2 observations, \mathbf{X} ($m \times p$) contains p different CO₂ flux tracers. These tracers include terrestrial biosphere model (TBM) estimates of CO₂ fluxes and remote sensing vegetation indices that are known to correlate with patterns in CO₂ fluxes (Sect. S2). There are different columns of \mathbf{X} corresponding to each CO₂ flux tracer in each different month and each different global region; we run the regression on all months simultaneously. These tracers (both the TBMs and vegetation indices) are subsequently run through an atmospheric transport model $h()$, in this case the Parameterized Chemistry and Transport (PCTM) model (Kawa et al., 2004). The coefficients estimated as part of the regression ($\underline{\mathbf{b}}$, $n \times 1$) scale these model outputs to best match the observations (\underline{z}). Furthermore, $\underline{\mathbf{b}}$ ($n \times 1$) is the model spinup or CO₂ mixing ratios at the beginning of the experiments, and $\underline{\epsilon}$ ($n \times 1$) are the model-data residuals.

We pair this regression with model selection; model selection will determine which combination of model outputs (i.e., columns of $h(\mathbf{X})$) best describe variability in current OCO-2 observations. It will identify the set of model outputs with the greatest power to describe the data and ensures that the regression does not overfit the data (e.g., Zucchini, 2000). We specifically implement model selection based on the Bayesian Information Criterion (BIC), one of the most commonly-used forms of model selection (Schwarz, 1978; Mueller et al., 2010; Gourdjii et al., 2012). We calculate a BIC score for many different combinations of model outputs, and each combination has a different set of columns ($h(\mathbf{X})$). The best combination has the lowest BIC score:

$$\underline{BIC} = L + p \ln(n^*) \quad (\text{S2})$$

where L is the log likelihood of a specific combination of model outputs, p is the number of model outputs in that combination, and n^* is the effective number of independent observations from OCO-2 during the study period. The log likelihood equation rewards combinations of model outputs that improve model-data fit, described in detail in Miller et al. (2018). By contrast, the second term in the equation ($p \ln n^*$) penalizes combinations with a greater number of model outputs, and it ensures that the selected combination is not an over-fit. This penalty and the log likelihood (L) not only depend upon the number of model outputs but also the effective number of independent observations (n^*). This number reflects the level of spatial and temporal correlation in the observational and model errors. If the spatial and temporal error correlations are large (i.e., bias-type errors), then the n^* will be small relative to the total number of OCO-2 observations. By contrast, if the errors are uncorrelated and completely independent, then n^* will equal the total number of OCO-2 observations. The companion paper Miller et al. (2018) describes in detail how we estimate this quantity.

S2 Additional detail on the tracers used in model selection

This section provides additional detail on the TBMs and vegetation indices that are used in the model selection experiments. These TBMs and vegetation indices are used as the input tracers in PCTM. We then generate forward atmospheric model simulations using PCTM and interpolate these model outputs to the locations and times of the OCO-2 observations to generate modeled XCO₂ total columns. These modeled columns become the columns of $h(\mathbf{X})$ in the model selection experiments (Eq. S1). Note that the multiple regression will scale the magnitude of the TBMs and vegetation indices in each region and each month to best match the observations (Eq. S1). As a result of this setup, the overall magnitude of each TBM and of each vegetation index does not affect the model selection results. Rather, this study assesses the degree to which the spatial and temporal patterns in the TBMs and vegetation indices, after being transported through the atmosphere to the times and location of OCO-2 observations, can explain the spatial and temporal patterns in OCO-2 observations.

We include four TBMs from the recent MsTMIP project (Huntzinger et al., 2013). These TBMs have very different space-time patterns and therefore represent a wide range of plausible flux patterns. The TBMs include the Dynamic Land Ecosystem Model (DLEM; e.g., Tian et al., 2011), the Lund-Potsdam-Jena Model Wald Schnee und Landschaft version (LPJ; e.g., Sitch et al., 2003), the Global Terrestrial Ecosystem Carbon Model (GTEC; e.g., King et al., 1997), and the Simple Biosphere Model with the Carnegie-Ames-Stanford Approach (SIBCASA; e.g., Schaefer et al., 2008). The original MsTMIP products have a spatial resolution of 0.5° latitude by 0.5° longitude, and we regrid these products to the PCTM model grid (1° latitude by 1.25° longitude). Furthermore, Fisher et al. (2016) downscaled the MsTMIP products to a 3-hourly temporal resolution; we use this version of the MsTMIP products in the present study.

The MsTMIP estimates are available through year 2010. Because these estimates are not available for the years of this study (2014-2015), we use a multi-year average as inputs in the PCTM model. Specifically, downscaled MsTMIP products are available from Fisher et al. (2016) for years 2004-2010, and we average the MsTMIP models over those years within each separate model grid box and for each separate 3-hourly time period to produce a multi-year average for each MsTMIP estimate. The resulting CO₂ flux estimates vary hour to hour and day to day but not year to year. Note that some recent inverse modeling studies using OCO-2 observations incorporate a prior flux estimate that has been generated for more recent years (e.g., Crowell et al., 2019). Unlike inverse modeling studies that often require a single prior flux estimate, we require numerous 3-hourly CO₂ flux tracers that represent a wide range of plausible patterns for the statistical model used in this study. The creation of a new, updated TBM inter-comparison is beyond the scope of this study. Furthermore, the objective of this study is to compare how the CO₂ flux constraint has improved as the retrievals have evolved from version 7 to versions 8 and 9. To facilitate this comparison, we have used the same set of flux models from MsTMIP as in the preceding companion paper (Miller et al., 2018).

In addition to these TBMs, we also utilize several vegetation indices as possible tracers of CO₂ fluxes within the regression (\mathbf{X} in Eq. S1). These include the enhanced vegetation index (EVI), normalized difference vegetation index (NDVI), and solar-induced fluorescence (SIF). Numerous studies indicate that biospheric CO₂ fluxes correlate with these vegetation indices – with EVI (e.g., Sims et al., 2008; Wu et al., 2011), NDVI (e.g., Cihlar et al., 1992; Wylie et al., 2003), and SIF (e.g., Guanter et al., 2014; Yang et al., 2015; Shiga et al., 2018). These indices are therefore good candidate CO₂ flux tracers to use within the model selection experiments.

We specifically use EVI and NDVI estimates from the Moderate Resolution Imaging Spectroradiometer (MODIS) Aqua product MYD13C1 (Didan, 2015a) and the MODIS Terra product MOD13C1 (Didan, 2015b). These products are collectively available at 8-day intervals. The individual Aqua and Terra products are each available at 16-day intervals. However, the two products are staggered, so Aqua and Terra can be combined to produce EVI and NDVI estimates every

8 days. These products have a 0.05° latitude by 0.05° longitude, and we regrid them to the PCTM model grid (1° latitude by 1.25° longitude). Both of these products are available for 2014 and 2015, the time period of this study.

We also use level 2 SIF retrievals from the Global Ozone Monitoring Experiment-2 (GOME-2) (Joiner, 2014). We convert the level 2 retrievals to a gridded SIF product using a block kriging method described by Tadić et al. (2017). This gridded product has a daily temporal resolution and the same spatial resolution as PCTM. We use this product as an input to the PCTM model and incorporate the resulting model outputs as candidate variables in the $h(\mathbf{X})$ matrix.

S3 Differences in the model selection results for versions 8 and 9 of the observations

The model selection results using versions 8 and 9 of the observations are very similar but exhibit a few subtle differences (Fig. 3 and 4). Specifically, we select slightly fewer CO_2 flux tracers using version 9 than version 8 in Fig. 3. These small differences are due to the stochastic nature of the statistical model. The regression model used in this manuscript requires an estimate of error variances and estimates of the error correlation length and correlation time. These estimates are used to calculate n^* (Eq. S2). We estimate these parameters using a randomized sub-selection of the observations due to the very large size of the OCO-2 dataset, a procedure described in Miller et al. (2018). The results of the regression analysis therefore exhibit a subtle stochasticity depending upon which observations were randomly selected for the variance and covariance estimation. For example, when we re-run the analysis in Fig. 3, we sometimes select a flux model in one or two more months using version 9 relative to version 8 and sometimes obtain identical results using versions 8 and 9.

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