Reply to reviewer 2:

In this manuscript, an alternative a priori flux constraint is presented in the context of a global CO_2 flux inversion performed using an ensemble Kalman filter (EnKF) with a short assimilation window. Observing system simulation studies (OSSEs) are preformed to give an idea of how this alternative constraint might function when used with real data in a real inversion. The flavor of EnKF used is the local ensemble transform Kalman filter (LETKF), as implemented in the Carbon in Ocean–Land–Atmosphere (COLA) data assimilation system, a global CO_2 flux inversion based on the GEOS-Chem transport model.

The alternative flux constraint is formulated in terms of the spatial gradient of the fluxes: finite differences of flux using adjacent grid boxes in the model. These spatial gradients are then added as new measurements in the measurement vector, as opposed to additional constraints in the traditional a priori state vector. Gradients used in this manner could capture the bulk of the flux constraint (its spatial and temporal patterns), while at the same time cutting the tie to the absolute value of the flux -- i.e. its overall constant offset or long-term mean. This in turn could be useful when using priors for which the variability is more robust than the long-term mean -- for example, the terrestrial biosphere models used as priors for CO_2 fluxes over land in global flux inversions, which do a good job getting the seasonality of the fluxes right (e.g., using satellite measurements vegetation greenness, plus assumptions on the timing of respiration) but a less-good job of estimating the integrated flux across a full year. By getting rid of the constraint to the long-term mean of the prior, the flux estimate might be freer to move to the long-term mean given by the data and not suffer from being biased in the direction of the incorrect or inaccurate prior. This of course would be at the cost of losing any benefit that that long-term prior mean might provide. In general, a flux constraint of this nature should be able to be implemented as a measurement in the measurement vector, as is done here, assuming that the measurement uncertainty used gives the constraint the same weight as it would have had if it had been implemented more traditionally in the a priori state vector. One would have to avoid double counting by not also having the traditional flux prior in force at the same time.

In their OSSE experiments, the authors compare the effectiveness of this flux spatial gradient constraint against the usual prior flux constraint (i.e. in terms of the actual flux value itself, not the spatial gradient) implemented either in the measurement vector or, more traditionally, as part of the a priori state vector; in the latter case, a couple different forms for the first guess of the flux at the new measurement time are used: either 1) a combination of the prior flux at the given time plus the flux estimate from the EnKF at the two immediately-earlier times, or 2) just the prior flux at the new time. This is done using one land biospheric model (VEGAS) to generate the 'true' measurements, and a second model (CASA) to be used as the prior flux. The authors find that, in general, when the flux gradient prior is used, the EnKF does a better job estimating the true fluxes than when three other approaches based on the absolute fluxes themselves (i.e., not gradients) are used.

While these results look promising, there are some inconsistencies in the results that I would like explained. Also, I suggest modified OSSEs in which the ocean fluxes are allowed to be corrected along with the land fluxes, in order to give a more realistic test of the new constraint. Finally, there is a lack of detail in the description of the methods used that makes it difficult for me as a reviewer to assess the full meaning of the results. I suspect that the general reader will have similar questions. I suggest that the authors add these needed details to the manuscript, address the points that I raise below, and resubmit, at which point I will re-review it and decide on final publication.

Reply: Many thanks for your constructive comments/suggestions and recognizing the AAPO method. We acknowledge that we have missed some important information and the experiments are not optimal. We are sorry for the inconvenience. We have reworked the manuscript in terms of method, experiment setup, and results. And the manuscript was also polished by AJE. The main changes are as follows:

1. Information: Adding more details about the short assimilation window and long observation window / experiment setup of initial condition, ensemble size etc. / observation localization / additive inflation / generation of pseudo observation.
2. Clearer method description: a) Assimilating CO_2 observation before assimilating a priori (Fig. 1). b) Using $\nabla\mathbf{f}$ to represent the spatial gradient.
3. New experiment setup: a) OCO2+insitu vs insitu only. b) Making sure the weight of a priori is identical in different experiments. c) Changing CASA to SiB4 as the a priori.
4. Clearer message from the OSSE results: Better hemispheric flux estimates using $\nabla\mathbf{f}$ in both experiments of assimilate OCO2+insitu or insitu only.

We hope that your major concerns are clarified and addressed. Note that we have made large revision on this manuscript that some parts of this paper are deleted or replaced (e.g., results section). Some sentences you commented on may be deleted. We are sorry about that, but these modifications are mainly based on your major concerns.

Comments:

First, the authors should describe in detail [with equations] the meaning of the terms 'assimilation window' and observation window', since how these terms are used in the context of the LETKF is not generally known. The reader should not have to go back to the previous LETKF papers to find this. Does the 1-day assimilation window mean that the filter is stepped forward in time a day at a time, each day allowing the new measurements to update the fluxes across the 7-day measurement window (i.e. the current day plus six previous days)? If so, the weight given to the flux constraint (or flux prior constraint) for each of those 7 days ought to be reduced, so that the integrated effect of the seven days of measurement updates affecting the fluxes on a given day is equivalent to the weight given to a single days' flux prior in some other estimation method (e.g. a variational method or a matrix-inversion-based Bayesian synthesis method).

Reply: Many thanks for your suggestions. We have added descriptions on the assimilation/observation window setup (Line 89) and guide the readers to refer Liu et al. (2019) for more details.

In this window steup, the persistent flux parameter and dynamic CO_2 state are updated on a daily basis using observations within the long observation window (7 days). To achieve that, for each analysis cycle, GEOS-Chem forecasts for 7 days to generate forecast observations, which are then assimilated with the corresponding observations using LETKF. This optimization process updates the model state (CO_2) and parameters (SCFs) at the end of the assimilation window, serving as the forecast initial conditions and timing for the subsequent analysis cycle. A comprehensive description of this unique LETKF feature can be found in the work of (Liu et al., 2019).

We intend to add an equation to illustrate it, but we find it may add more questions to the readers. The LETKF analysis equation is,

$$\bar{\mathbf{x}}^{a}_{t_1} = \bar{\mathbf{x}}^{b}_{t_1} + \mathbf{X}^{b}_{t_1}\widetilde{\mathbf{P}}^{a}\left(\mathbf{Y}^{b}_{t_0\to t_7}\right)^{T}\mathbf{R}^{-1}_{t_0\to t_7}\left(\mathbf{y}^{o}_{t_0\to t_7} - \bar{\mathbf{y}}^{b}_{t_0\to t_7}\right)$$

$$\widetilde{\mathbf{P}}^{\mathbf{a}} = [\left(\mathbf{Y}^{b}_{t_0\to t_7}\right)^{T}\mathbf{R}^{-1}_{t_0\to t_7}\left(\mathbf{Y}^{b}_{t_0\to t_7}\right) + (K-1)\mathbf{I}]^{-1}$$

where the flux parameter $\mathbf{f}$ is augmented to the CO_2 state $\mathbf{c}$ that $\mathbf{x} = [\mathbf{c}, \mathbf{f}]^{\mathbf{T}}$; the superscripts a and b denote the analysis and background (first guess), respectively; $\bar{\mathbf{x}}$ and $\mathbf{X}$ are the ensemble mean and ensemble perturbation, respectively; the subscript t_1 indicate the end of assimilation window of 1 day; $\mathbf{y}^{o}_{t_0 \to t_7}$ is the CO_2 observations within the observation window of 7 days; $\mathbf{y}^{b}_{t_0 \to t_7}$ is the forecasted observations corresponding to each observations; $\mathbf{Y}^{b}$ is the ensemble perturbation in the observation space; $\mathbf{R}$ is the observation error matrix; $\widetilde{\mathbf{P}}^{a}$ is the analysis error covariance; K is the ensemble size which is set to 20; and $\mathbf{I}$ is the identical matrix.

In the LETKF analysis equation, the windows are expressed by the subscripts, readers may misunderstand that there are only 7 timesteps of observations. We have discussed for several time and decide not putting it in the manuscript but describing it directly.

Second, the weights given to the spatial gradient constraint in the inversion relative to the straight flux constraint cases ought to be given. Perhaps the spatial gradient case does a better job because it has a looser (or tighter) weighting than the other cases. A tighter flux prior usually results in a worse fit to the measurement data; or, vice versa, the inversion can over-fit the measurement data at the cost of too great a change from the flux prior. Knowing the weights assumed in the inversion for the gradient case vis a vis the straight flux case could help assess this. Similarly, some information on how good the fit to the measurement data is for the four cases could help.

Reply: Thanks for the comments. We fully agree with the reviewer that the weight of a priori in different experiments should be identical. Since we assume that the uncertainty of the two a priori (flux and its spatial gradient) is 5 time larger than than the analysis uncertainty (Text A1, Line 308). To further illustrate the weight of the a priori, figure R1 shows the uncertainty reduced by the CO_2 observation and the a priori in different experiments, which varified that the weight of the two a priori are identical in EXP-GOI (spatial gradient) and EXP-FOI (flux). The ensemble uncertainty reduciton (EUR) is defined as,

$$\mathbf{EUR}_{i,t} = \frac{\boldsymbol{\sigma}^{b}_{i,t} - \boldsymbol{\sigma}^{a}_{i,t}}{\boldsymbol{\sigma}^{b}_{i,t}},$$

where $\boldsymbol{\sigma}^{b}_{i,t}$ and $\boldsymbol{\sigma}^{a}_{i,t}$ is the first guess and final analysis ensemble uncertainty, respectively, at a given grid point i and a given time t. Since there are two types of observation, the EUR can be separated to two parts of EUR^{CO2} and EUR^{Ap} as,

$$\mathbf{EUR}^{CO2}_{i,t} = \frac{\boldsymbol{\sigma}^{b}_{i,t} - \boldsymbol{\sigma}^{a*}_{i,t}}{\boldsymbol{\sigma}^{b}_{i,t}},$$

$$\mathbf{EUR}^{Ap}_{i,t} = \frac{\boldsymbol{\sigma}^{a*}_{i,t} - \boldsymbol{\sigma}^{a}_{i,t}}{\boldsymbol{\sigma}^{b}_{i,t}},$$

where the superscript $a*$ denote the analysis after assimilating CO_2 observation; the superscript Ap denotes the a priori.

As show in Figure R1, for EXP-GOI, the EUR^{CO2} in the northern middle and high latitudes of North America and Europe, where the CO_2 observation network is dense, can exceed 30%. Generally, the EUR^{CO2} decreases from north to south. In South America and Africa, the EUR^{CO2} is around 10%. Since the uncertainty of a priori is set to be proportional to the ensemble uncertainty, ***EUR^{Ap} is approximately 5% and almost identical at different grids. For EXP-FOI, the EUR^{Ap} is configured to be identical to EXP-GOI; thus, the weights of a priori in EXP-GOI and EXP-FOI are expected to be identical.*** However, in EXP-GOI, the EUR^{Ap} in the Qinghai-Tibet Plateau, Andes, Sahel, and Arabian Plateau is relatively larger than in the other areas, suggesting that, even though the error of the gradient at different grid points is identical, the EUR^{Ap} is also affected by the geography. In EXP-GI, which assimilated only the in-situ data, the EUR^{CO2} is approximately half that in EXP-GOI, resulting in similar EUR^{CO2} and EUR^{Ap} in South America and Africa.

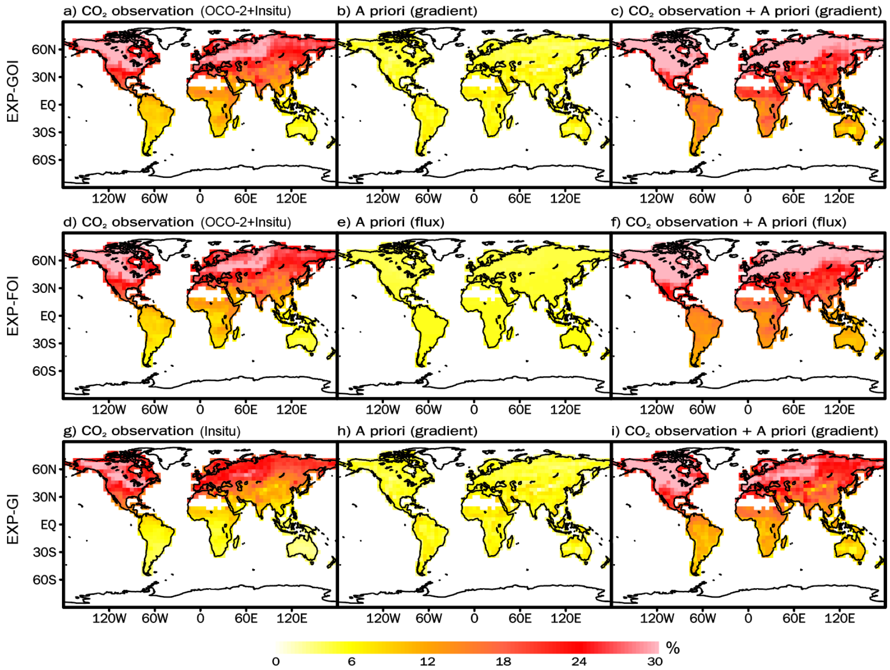

Figure R1: a-c) The ensemble uncertainty reduction in EXP-GOI from the satellite and in-situ CO_2 observations, the a priori of the gradient, and the sum of the former two. d-f) The ensemble uncertainty reduction in EXP-FOI from the satellite and in-situ CO_2 observations, the a priori of the original flux, and the sum of the former two. g-i) The ensemble uncertainty reduction in EXP-GOI from the in-situ CO_2 observations, the a priori of the gradient, and the sum of the former two.

Third, if the flux constraint can be implemented equally as well in the measurement vector as in the a priori state vector, then the two cases in which the straight flux prior are implemented these two ways should give the same flux results. That is, the EXP-NP case, in which the flux prior is applied normally, as the a priori constraint on the fluxes in the state vector, and the EXP-AP case, in which the flux prior is assimilated as a measurement in the measurement vector, should give the same flux estimates. But they don't -- they give quite different answers, as seen by the turquois and orange lines in Figures 3 through 5. What is it about the different implementation of the prior that causes these differences? Different weights used in each case? A different number of times that the constraint is applied (if fluxes at multiple times are updated by measurements at a single time)? Similarly in Figures 6 and 7, the EXP-NP case gives much worse RMSEs for flux and flux spatial gradient than does EXP-AP. Why is this, if the two ways of implementing the prior are equivalent? I can understand why, with a short-window inversion, the EXP-NP case might have higher values for these metrics (i.e. a flux error frozen in at a given assimilation step would need to be corrected by a balancing error at the next step of opposite sign, resulting in a lot of noise in time), but what is it about the EXP-AP implementation that prevents this?

Reply: Thanks for the comments. The reviewer may misunderstand the experiment name. The EXP-NP (now EXP-OI) is the experiment that does not use a priori. The much worse RMSEs in EXP-NP is because of lacking regularization. The cases that using the a priori flux in the measurement vector is EXP-P. And comparing between EXP-AP and EXP-P, there differences are small.

The case using the a priori flux in the measurement vector has several differences as compared to the case using the a priori flux in the a priori vector. Since the AAPO method treat the a priori as a special observation, the a priori can reduce the ensemble uncertainty as show in Figure R1, thus will change the values of each ensemble member. However, when placed in the a priori vector, only the ensemble mean is changed, and the ensemble uncertainty are not reduced.

Furthermore, the two cases are not comparable in terms of weight. The measurement vector case applied observation localization with a small radiu, thus the surrounding a priori information will also influence the local flux estimates. Thus, it is hard for us to make the two cases identical in terms of weight. Considering this point, we decide to delete the case that using the a priori flux in the measurement vector.

Fourth, because the OSSE experiments use the same ocean fluxes in the truth and assimilation runs, there is effectively no error coming from the oceans and no need to allocate any flux corrections there in the inversions. This is effectively the same thing as holding the oceans fixed and only allowing flux changes over the land areas. This significantly simplifies the inversion and gives an overlyoptimistic view of how well the inversions can retrieve the land fluxes. However, even worse, it may favor the spatial gradient prior constraint more than the straight flux prior constraint, since, with the ocean corrections fixed to zero, the fluxes bordering the oceans are then strongly constrained by the spatial gradient constraint, and the fluxes in the interior similarly prevented from moving as much as they otherwise would. With the straight flux constraint, however, the fluxes are still allowed to trade off corrections between continents. It would be interesting to see whether these same favorable results with the EXP-ASG case are achieved if more realistic errors are allowed over the oceans (i.e., if separate ocean flux models were used in generating the truth and prior, as has been done with the land biospheric fluxes here).

Reply: Thanks for the comments and suggestions. We agree with the reviewer that the ocean flux plays an important role in regulating the global carbon cycle, and considering the errors from the ocean will make the OSSEs more realistic. But for an OSSE that designed for validating the AAPO method, the main conclusion that the spatial gradient is better than the flux itself holds when focusing on the land. And some previous OSSE studies do not consider the error from the ocean (e.g., Liu et al., 2014).

Moreover, we did not consider the error from ocean because of the short window feature of COLA. Current bottom-up ocean carbon flux estimates usually report only monthly mean value which does not fit well with the additive inflation step in COLA. The additive inflation requires daily bottom-up estimates. And in real data assimilation experiments, COLA uses a daily ocean carbon flux estimates from Jena Carboscope (Rödenbeck et al., 2014) as the a priori ocean flux. And, to our best knowledge, we do not know other public-available daily ocean flux product (except the CMIP output), which is not practical for us to use another independent daily ocean flux product as the a priori.

As the reviewer point out that the ocean flux may favor the spatial gradient of flux. We are investigating it in the real data assimilation experiments that using the Jena Carboscope estimates as the a priori ocean flux.

Reference:

Rödenbeck, Christian, et al. "Interannual sea–air CO2 flux variability from an observation-driven ocean mixed-layer scheme." Biogeosciences 11.17 (2014): 4599-4613.

Liu, Junjie, et al. "Carbon monitoring system flux estimation and attribution: impact of ACOS-GOSAT XCO2 sampling on the inference of terrestrial biospheric sources and sinks." Tellus B: Chemical and Physical Meteorology 66.1 (2014): 22486.

Fifth, it would be useful for the authors to discuss how specific their results are to the flux inversion method they use (a short-window EnKF). Would they anticipate that the alternative flux spatial gradient constraint would give similar improvements in methods that allow the transport model to link measurements and flux corrections across a longer span? Similarly, since this reliance on the transport model is less important when there is more data coverage, would the results obtained here still hold were a less-dense observing network (the in situ CO2 network instead of a CO2-measuring satellite, say) to be used?

Reply: Thanks for the suggestions. To answer this question, we conducted extra two experiments (EXP-GI and EXP-FI) that assimilates only the insitu observations.

First, we acknowledge that the short-window based COLA system may not be better than long window-based systems while assimilate only the insitu observations (Line 247): *Since the observation window in COLA is relatively shorter than some traditional systems (e.g., CarbonTracker, UoE, and CAMS), we speculate that long window-based systems should be more suitable for inversions using only surface* CO_2 *observations and constrained by the a priori* F_{TA}.

However, comparing EXP-GI and EXP-FI, the main conclusions still hold. The hemispheric partitioning estimates in EXP-GI is less biased even only constrained by the insitu observations. And the seasonal RMSEs in EXP-GI are also smaller.

More-detailed comments:

14: “dynamic constraints” I do not believe that the reason the inversion problem is ill-posed is because of the lack of explicit dynamical constraints in the setup. Really it is due to the sparse data.

Reply: Thanks for the comments. We have deleted the "dynamic constraints" in the abstract.

16-17: "Ensemble Kalman filter-based inversion algorithms usually weigh a priori flux to the background or directly replace the background with the a priori flux." It is not very clear what this means. Please reword. What do you mean by ‘background’?

Reply: Thanks for the comments. The ‘background’ corresponds to the first guess. In this context maybe misleading and reader may refer to the ‘background’ CO_2 concentration. Thus, we replace the ‘background’ to ‘first guess’.

21: spell out "AAPO"? It is not clear why you use this combination of letters for what you are describing.

Reply: Thanks for the comment. We have spell out “AAPO” in the abstract in Line 24, “Assimilates A Priori information as a special Observation (AAPO)”.

38: I wouldn't say the problem is ‘ill-posed’ because of transport errors or retrieval biases -- those just bias the result. Ill-posedness is more due to lack of a sufficient data constraint, for example, trying to solve for more unknowns than can be constrained by a given number of data points.

Reply: Thanks for the comment. We agree that the systematic errors are not the reason of being “ill-posed” but other influence factors. The sentences are revised to be clearer in Line 42, “*However, the top-down estimation could be ill-posed because of the sparseness feature of atmospheric* CO_2 *observations. And systematic errors in the transport model and satellite retrieval can contaminate the illustration of inferred SCFs (Basu et al., 2018; O'Dell et al., 2018; Yu et al., 2018; Schuh et al., 2019)*”.

49: "the LETKF with a short assimilation window and long observation window setting" I do not see this described later in the text. Please describe what these ‘window’ terms refer to, for example in terms of the filter time stepping, what span of data is assimilated at each time step, and what span of fluxes is allowed to change per time step; preferably with equations.

Reply: Thanks for the comment on the windows. We have added more details on describing the windows from Line 88 to Line 95. The end of assimilation window means when update the state and parameter. Within the observation window, the model will forecast the modeled observations in order to match with the 7 days of observations.

54-56: "On the other hand, even though a priori information includes biases, it could be used to further improve the SCF estimation in COLA because it includes important dynamic information generated by terrestrial models, which is missing in the top-down inversion system." It is not clear why you think that dynamic information generated by the terrestrial models is not represented in the top-down inversion systems. Insofar as it is used to generate the a priori SCFs, it is in there. Do you mean to say that the dynamical constraint of the a priori fluxes is not represented explicitly as a dynamic model in the Kalman filter, i.e. as a formal constraint?

Reply: Thanks for the comment and pointing out the mistake. Yes, we intend to say that the ensemble-based COLA system does not hold a dynamic model and a priori can partly compensate the dynamic information.

We revised this sentence to be more accurate in Line 60, " *On the other hand, since the ensemble-based COLA system does not hold a dynamic flux model, a priori fluxes generated by terrestrial models has the potential to further enhance the SCFs estimation in the COLA system*".

75: add "at" after "including"

Reply: Thanks for pointing out the mistake. To make this sentence clearer, we have revised this sentence, "*LETKF is a deterministic variation of EnKF and is known for its efficiency in DA.*".

77-81" Similar to the other EnKF, the LETKF prefers a short assimilation window to produce accurate model state analysis, which reduces noise within the background for parameter estimation. On the other hand, parameter estimation requires a long training period to enhance the model response to the estimated parameter (the signal). Therefore, COLA implements a new version of LETKF with a unique feature of a short assimilation window (1 day) and a long observation window (7 days) to enhance the SCF estimation (Liu et al., 2019)." It is not clear how these various 'windows' relate to the fluxes being solved for. You should write out with equations what is being solved for, how the time stepping is done, what observations are assimilated in which time step with which weights, etc. And point out which spans are the 'observation window' versus the 'assimilation window'. This may be detailed in previous LETKF papers, but the reader shouldn't have to go back to them to understand what is being used here.

Reply: Thanks for the comment on the windows. We have added more details on describing the windows from Line 88 to Line 95. The end of assimilation window means when update the state and parameter. Within the observation window, the model will forecast the modeled observations in order to match with the 7 days of observations. We intend to add an equation to illustrate it, but we find it may add more questions to the readers. The LETKF analysis equation is,

$$\bar{\mathbf{x}}^{a}_{t_1} = \bar{\mathbf{x}}^{b}_{t_1} + \mathbf{X}^{b}_{t_1}\widetilde{\mathbf{P}}^{a}\left(\mathbf{Y}^{b}_{t_0\to t_7}\right)^{\mathrm{T}}\mathbf{R}^{-1}_{t_0\to t_7}\left(\mathbf{y}^{o}_{t_0\to t_7} - \bar{\mathbf{y}}^{b}_{t_0\to t_7}\right)$$

$$\widetilde{\mathbf{P}}^{\mathbf{a}} = [\left(\mathbf{Y}^{b}_{t_0\to t_7}\right)^{\mathrm{T}}\mathbf{R}^{-1}_{t_0\to t_7}\left(\mathbf{Y}^{b}_{t_0\to t_7}\right) + (\mathrm{K}-1)\mathbf{I}]^{-1}$$

where the flux parameter $\mathbf{f}$ is augmented to the CO_2 state $\mathbf{c}$ that $\mathbf{x} = [\mathbf{c}, \mathbf{f}]^{\mathbf{T}}$; the superscripts a and b denote the analysis and background (first guess), respectively; $\bar{\mathbf{x}}$ and $\mathbf{X}$ are the ensemble mean and ensemble perturbation, respectively; the subscript t_1 indicate the end of assimilation window of 1 day; $\mathbf{y}^{o}_{t_0\to t_7}$ is the CO_2 observations within the observation window of 7 days; $\mathbf{y}^{b}_{t_0\to t_7}$ is the forecasted observations corresponding to each observations; $\mathbf{Y}^{b}$ is the ensemble perturbation in the observation space; $\mathbf{R}$ is the observation error matrix; $\widetilde{\mathbf{P}}^{a}$ is the analysis error covariance; K is the ensemble size which is set to 20; and $\mathbf{I}$ is the identical matrix.

In the LETKF analysis equation, the windows are expressed by the subscripts, readers may misunderstand that there are only 7 timesteps of observations. We have discussed for several time and decide not put it in the manuscript but describing it directly. The descriptions in Line 88 are, "*In this approach, the persistent flux parameter and dynamic CO_2 state are updated on a daily basis using observations within the long observation window (7 days). To achieve that, for each analysis cycle, GEOS-Chem forecasts for 7 days to generate forecast observations, which are then assimilated with the corresponding observations using LETKF. This optimization process updates the model state (CO_2) and parameters (SCFs) at the end of the assimilation window, serving as the forecast initial conditions and timing for the subsequent analysis cycle*".

119: "In COLA, the main purpose of applying a priori regularization is to introduce the dynamic constraint for SCF estimation." It is not at all clear that you have now introduced a better dynamic constraint by changing from using the prior flux value to using spatial gradients instead. Nothing involving dynamics has been changed by this. All you have succeeded in doing is removing the link to the overall absolute value of the prior flux (the long-term mean). That may indeed have value, but don't confuse it with dynamics. Any dynamics that were or were not in the original flux prior are still there with this new constraint. Please reword to reflect this, here and elsewhere in the document where 'dynamics' are discussed.

Reply: Thanks for the comment. In the last version, we intended to use 'dynamic/dynamically' to describe that the added a priori information may partly compensate the loss of a priori fluxes in COLA. The a priori fluxes are generated using dynamic vegetation model, thus the a priori fluxes themselves contains dynamic information. In this context, we acknowledge that the description is very misleading. We have deleted the dynamic/dynamically in some places (e.g., the Title) and rewrite some sentences. For example, in Line 137, "*Within COLA, rather than using the SCFs estimation itself as the a priori information, we propose the utilization of the spatial gradient of a bottom-up estimation of SCFs ($\nabla \boldsymbol{f}$) as a more suitable alternative*".

138-147: You are free to add dynamical noise to your propagation of information forward in time in your model. You should discuss why you choose not to add dynamical noise that reflects errors in your transport model and/or variability in the land fluxes not captured by a forward propagation based on persistence. Why do you instead add an inflation term that is based more on the technical needs of your EnKF rather than a physically-based dynamical error?

Reply: Thanks for the comment. First, in the perfect model OSSEs, we did not consider the transport model error. We acknowlege that there is transport model error while conducting real data assimilation. If you want to consider or reduce the transport error, the error should be related to the transport model by perturbing the meteorology fields instead of the adding noises to the flux ensembles. The transport model error is always a tough question for CO_2 inversion. Several recent studies have discussed the impact of transport model error/differences on modeling the CO_2 concentration (Schuh et al., 2019, 2023). But those studies are performed in forward simulation and considering/reducing transport error in inversions needs to couple with an online general circulation model instead of an offline transport model (Kang et al., 2012).

Second, as the reviewer pointed out, the forward propagation based on the persistence can not capture the noise/uncertainty in the land fluxes. The additive inflation method is designed to add the uncertainty related to the land fluxes physically. We have added the details of the inflation method to the appendix section (Text A1). Based on the inflation method, the noises/variance are added based on the temporal changes of the a priori fluxes.

Reference:

Kang, Ji-Sun, et al. "Estimation of surface carbon fluxes with an advanced data assimilation

methodology." Journal of Geophysical Research: Atmospheres 117.D24 (2012).

149-150: "COLA assimilates the a priori SCF spatial gradients into the system, which needs to define the a priori uncertainty. In this study, we simply set the a priori uncertainty proportional to the uncertainty of the analysis ensemble uncertainty." Please describe what this analysis ensemble uncertainty looks like. Does it differentiate between forested areas that are likely to have larger fluxes and flux uncertainty and desert areas that are likely to have smaller ones? (Or similarly for flux gradients?) A sensitivity study done using uncertainties proportional to the magnitude of the fluxes in either the VEGAS or CASA models, or based on the difference between VEGAS and CASA (and preferably other models), would be welcome to test the dependence of your results on this assumption.

Reply: Thanks for the comment. Yes, the analysis uncertainty of flux or its spatial gradient is large in the northern forest areas and small in the desert. The magnitude of the analysis uncertainty is mainly dependent on the spatial coverage of CO_2 observation (Fig. R1) and the additive inflation method described in the appendix (Text A1). In area with more CO_2 observations and smaller monthly variation of fluxes, the analysis uncertainty would be smaller. With the details on the additive inflation method, we hope that your questions on the analysis ensemble uncertainty are addressed.

The sensitivity test suggested by the reviewer is interesting. We plan to test these configurations in the future. We discussed the choose of a priori uncertainty in Text A1 (Line 350), "*In reality, a bottom-up SCFs estimation product may come with its uncertainty estimation. We may derive the uncertainty of the SCFs spatial gradient from it. The importance and impact of those uncertainties and whether their accuracies are good enough for DA application remain to be further explored in the future*".

165-166: "We set the CO2 observation localization radius to 4000 kilometers." Since the general reader probably will not understand what this means, please say what this means, practically, in your inversion setup. Does it mean literally that each observation has zero impact on any flux farther away than 4000 kilometers at a given time? What about at previous times?

Reply: Thanks for the suggestion. Miyoshi et al. (2007) described the localization weight w(r) in LETKF as,

$$w(r) = e^{(\frac{{r_h}^2}{2{d_h}^2}+\frac{{r_v}^2}{2{d_v}^2})},$$

where d_h and d_v denote the horizontal and vertical localization radius; and r_h and r_v is the distance between an observation and a model grid horizontally and vertically. If the distance exceeds $2\sqrt{\frac{10}{3}}d$, the observation will be discarded. And we did not apply temporal localization.

We discussed and decided to put the details to the manuscript and explicit guiding reader to infer Miyoshi et al. (2007) for the information of localization scheme in Line 163.

168-174: By using the same fossil fuel, ocean, and wildfire fluxes in both the truth and prior, the simulation is artificially rosy: terrestrial fluxes are solved for using only differences there by permitting flux corrections only over the land and not over the ocean. By not considering the impact of ocean flux errors, this will give you lower error estimates for the land fluxes than you'd get otherwise. It would be a useful sensitivity study to look at the impact of considering ocean flux errors, as well. Figures 6 & 7: The difference between the EXP-NP and EXP-AP cases still needs to be explained. Yes, the short window of the COLA setup results in over-fitting of the data and noisy fluxes (and spatial gradients) in the EXP-NP case. But how does applying the prior flux constraint via the measurement vector prevent this?

Reply: Thanks for the comments. We agree with the reviewer that the ocean flux plays an important role in regulating the global carbon cycle and considering the errors from the ocean will make the OSSEs more realistic. But for an OSSE that designed for validating the AAPO method, the main conclusion that the spatial gradient is better than the flux itself holds when focusing on the land. And some previous OSSE studies do not consider the error from the ocean (e.g., Liu et al., 2014). Moreover, we did not consider the error from ocean because of the short window feature of COLA. Current bottom-up ocean carbon flux estimates usually report only monthly mean value which does not fit well with the additive inflation step in COLA. The additive inflation requires daily bottom-up estimates. And in real data assimilation experiments, COLA uses a daily ocean carbon flux estimates from Jena Carboscope (Rödenbeck et al., 2014) as the a priori ocean flux. And, to our best knowledge, we do not know other public-available daily ocean flux product (except the CMIP output), which is not practical for us to use another independent daily ocean flux product as the a priori. As the reviewer point out that the ocean flux may favor the spatial gradient of flux. We are investigating it in the real data assimilation experiments that using the Jena Carboscope estimates as the a priori ocean flux.

The reviewer may misunderstand the experiment name. The EXP-NP (now EXP-OI) is the experiment that does not use a priori. The much worse RMSEs in EXP-NP is because of lacking regularization. The cases that using the a priori flux in the measurement vector is EXP-P. And comparing between EXP-AP and EXP-P, there differences are small. The case using the a priori flux in the measurement vector has several differences as compared to the case using the a priori flux in the a priori vector. Since the AAPO method treat the a priori as a special observation, the a priori can reduce the ensemble uncertainty as show in Figure R1, thus will change the values of each ensemble member. However, when placed in the a priori vector, only the ensemble mean is changed, and the ensemble uncertainty are not reduced. Furthermore, the two cases are not comparable in terms of weight. The measurement vector case applied observation localization with a small radiu, thus the surrounding a priori information will also influence the local flux estimates. Thus, it is hard for us to make the two cases identical in terms of weight. Considering this point, we decide to delete the case that using the a priori flux in the measurement vector.

Reference:

Rödenbeck, Christian, et al. "Interannual sea–air CO2 flux variability from an observation-driven ocean mixed-layer scheme." Biogeosciences 11.17 (2014): 4599-4613.

Liu, Junjie, et al. "Carbon monitoring system flux estimation and attribution: impact of ACOS-GOSAT XCO2 sampling on the inference of terrestrial biospheric sources and sinks." Tellus B: Chemical and Physical Meteorology 66.1 (2014): 22486.

290: What does 'dynamically' in 'dynamically assimilated' indicate? Is this some special sort of assimilation method? Also, define what the acronym 'AAPO' refers to.

Reply: Thanks for the comment and pointing out the mistake. As the reviewer mentioned in the previous comments, the 'dynamically' may mislead readers. And we deleted it in Line 290. And 'AAPO' is defined in the method section. And we revised the sentense in Line 290, "*In this study, we developed a novel algorithm for the ensemble-based COLA CO_2 inversion system, in which the spatial gradient of a bottom-up model estimation is assimilated as a special observation*".

297-304: "However, the advantage of error transport is partly sacrificed or abandoned by introducing the a priori flux information to the background in most of the EnKF-based CO2 inversion methods (Peters et al., 2007; Feng et al., 2009). This is because of the loss of a dynamic model to provide the background and the background covariance estimations. Different from most EnKF-based systems, COLA maintains the mean and error transport advantages of the EnKF by including the dynamic information constraints of the a priori flux spatial gradient and using an additive covariance inflation method (Liu et al., 2022)." I agree that the loss of the dynamical model for the fluxes in most of our flux inversion methodologies

is unfortunate. I do not believe, however, that you are remedying that with your spatial gradient constraint here. Nothing has changed regarding the dynamics in using this constraint. Your only change is to cut the tie to the long-term mean, allowing your estimate to be shifted up or down as a whole more easily.
Reply: Thanks for the comments. We acknowledge that this description is exaggerated. We deleted this paragraph to avoid misunderstanding.
310: 'unique strategy'? Maybe referring to it as a 'new strategy' would be better.
Reply: Thanks for the comments. We have revised to "novel strategy".

Lists of new figures and table:

Table 1: Assimilation experiments setup.

Experiment	EXP-GOI	EXP-FOI	EXP-OI	EXP-GI	EXP-FI
A priori	∇f	f		∇f	f
Observation	OCO-2+In-situ	OCO-2+In-situ	OCO-2+In-situ	In-situ	In-situ

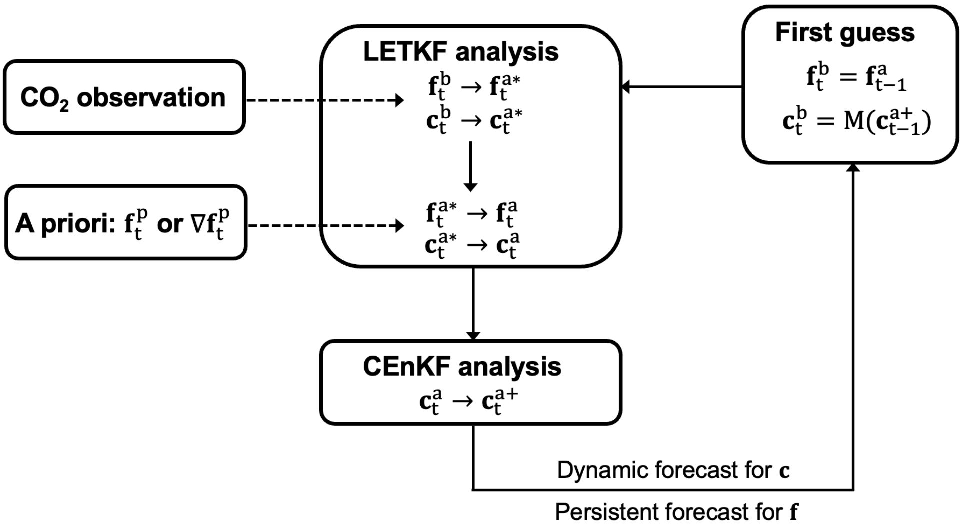

Figure 1: The assimilation cycle of the COLA system, illustrating how and where the a priori is assimilated.

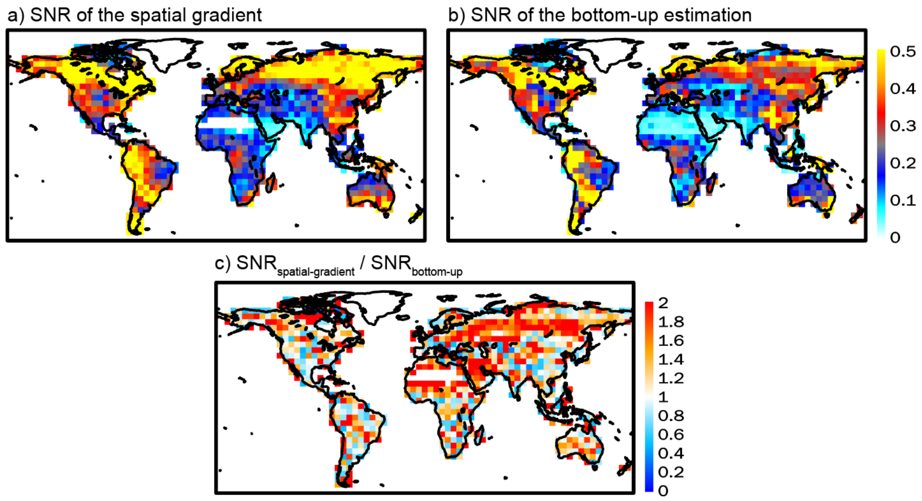

Figure 2: a) The annual mean signal-to-noise ratio pattern of the a priori F_{TA} spatial gradient. b) The same as a) but for the a priori F_{TA}. c) Annual mean signal-to-noise ratio of the spatial gradient divided by the signal-to-noise ratio of the F_{TA}.

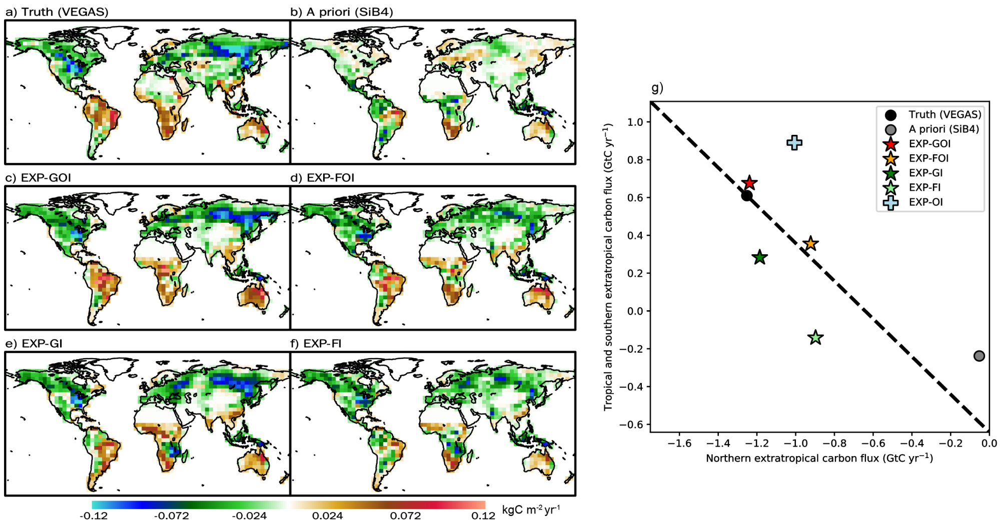

Figure 3: The annual mean F_{TA} in 2015 of a) the truth, b) the a priori, c) EXP-GOI, d) EXP-FOI, e) EXP-GI, and f) EXP-FI. g) Comparison of the annual total F_{TA} in the northern extratropical area and the tropical and southern extratropical areas. Different scatters denote the truth, the a priori, and the different experiments. The dashed black line denotes the global carbon budget.

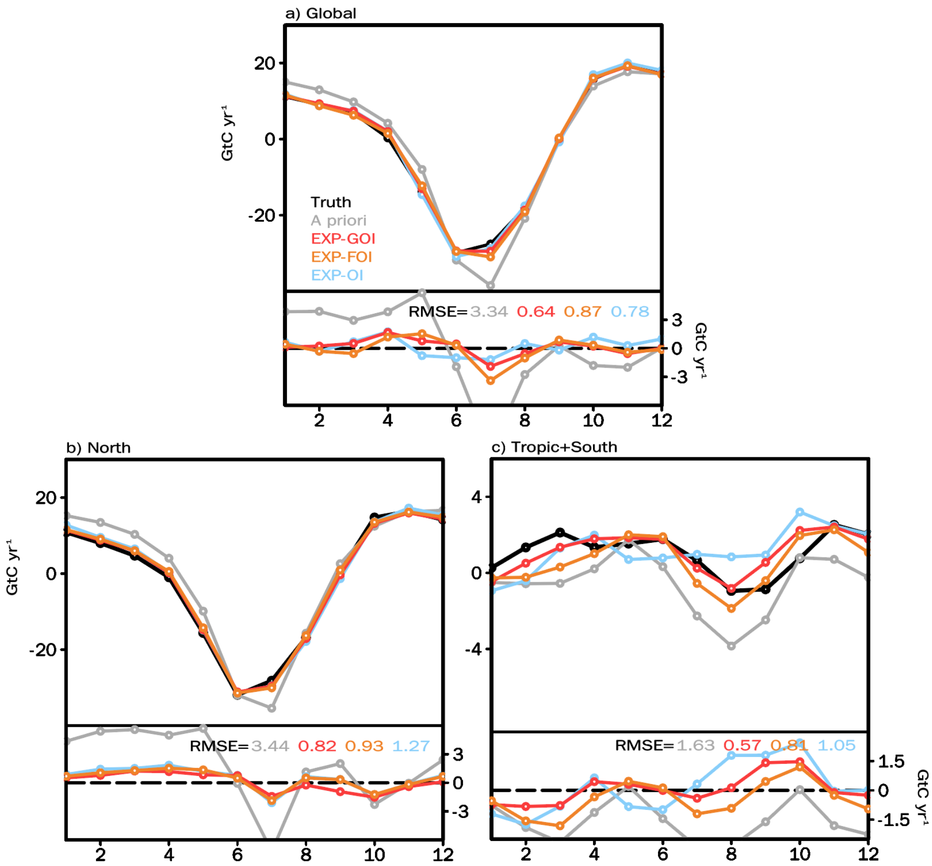

Figure 4: The top figures in each subplot are the a) global, b) northern extratropical, and c) tropical and southern extratropical seasonal cycles of F_{TA} in the truth (black), the a priori (gray), EXP-GOI (red), EXP-FOI (orange), and EXP-OI (sky blue). The bottom figures in each subplot are the global total difference of the a priori and the three assimilation experiments compared to the truth. The annual mean RMSEs of the a priori F_{TA} and the three experiments are denoted at the upper right corner of the bottom figures.

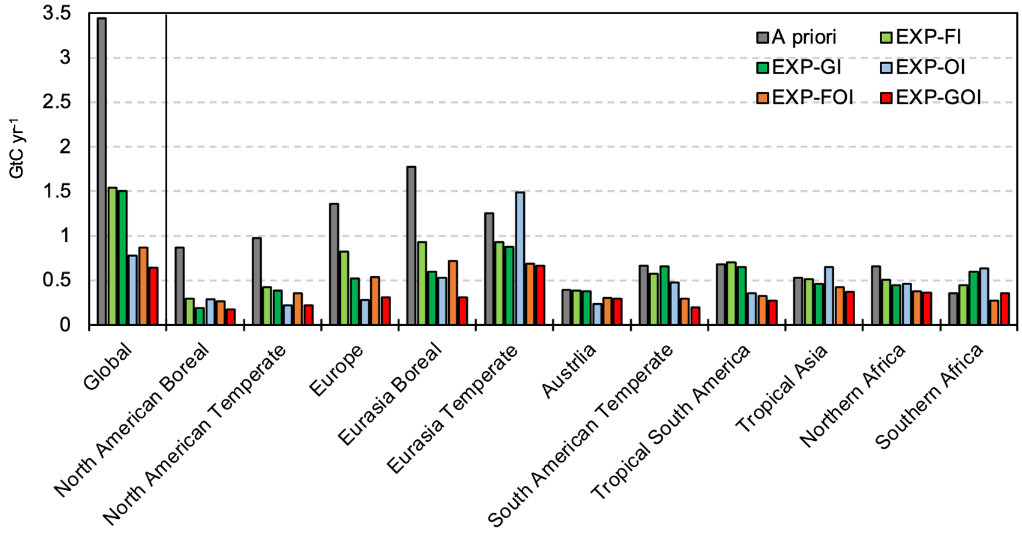

Figure 5: The regional RMSE of the a priori and the five assimilation experiments compared to the truth. The regions are defined by the OCO2MIP.