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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Regional-scale geostatistical inverse modeling of North American CO_2 fluxes: a synthetic data study" *by* S. M. Gourdji et al.

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Responses to Comments from R. Law, Referee #1

The authors thank the reviewer for her thoughtful suggestions to improve the quality of the manuscript. Responses to individual comments are included below. (Original referee comments are in italicized text.)

"***General comments***

The paper by Gourdji et al. presents a range of synthetic data inversions for continental North America using a geostatistical method. While the case presented is rather limited in its scope (only one summer month and one network of sites), the paper endeavours to identify general principles from this that might be applied in a wider range of cases. Iam concerned that the paper is too detailed and therefore too long, with the result that the most important findings tend to get lost. I would make two suggestions that might allow the manuscript to be reduced in length by 20%.

1) The authors remove some material that they consider to be less important. It seems to me that each of the tests they have performed is valid, but perhaps not everything needs to be presented? Deciding what can be left out of a paper is often as important as deciding what needs to go in a paper. Perhaps it is sufficient to just note that some of the tests were performed, with a single sentence to describe the main result. I realize this is already done to some extent, such as for the cases with and without night-time data, but I think there may be other places where a shorter presentation of the results may be justified. Some of the findings I thought were most interesting were the difficulty in estimating the spatial covariance when transport error was included, the impact of including temporal covariance in improving the uncertainty estimates and what seemed like rather poor results at the ecoregion scale compared with the earlier metrics used to assess the inversion. The authors may agree that these are worth highlighting or they may want to choose other points to focus on."

The authors agree that the discussion paper was overly long and it was easy to get lost in the details. Therefore, the authors are making the following modifications to the paper to improve readability, reduce redundant text, and generally make it easier to follow the flow of analysis.

1. The number of cases has been cut down from 6 to 3. These 3 cases focus on

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just the impact of temporal aggregation error on the flux side, and they all use the same 3-hourly concentration data vectors. The three presented flux intervals are 3-hourly, a 4-day average diurnal cycle (with 3-hourly resolution), and a full 4-day average. These new cases were chosen to help isolate one component of the changing setup for the inversion, i.e. temporal aggregation error, which seems especially relevant when using data with strong diurnal and synoptic variability. Also, it appears advantageous to use sub-daily measurement data when possible, at least in a pseudo-data setup without any systematic transport error, and therefore, we chose to not present the cases with daily or 8-day averaged concentrations in the revised manuscript. (These cases will still be mentioned briefly in the discussion, although specific results will not be presented in the revised manuscript.)

2. Section 4.2 focusing on how temporal aggregation error varies by case, tower and time of day will be substantially cut down and the associated figures (3 and 4) will be removed. These concepts will be briefly described in the text and used to inform the comparison of flux results.

3. RML-Inv parameters for **R** and **Q** are now estimated simultaneously. This is more technically correct than holding one set of parameters constant while optimizing the other set, as was done in the discussion paper. Also, optimized covariance parameters using RML-Inv will now be presented with and without simulated transport error.

4. All modifications to the covariance matrices for the "best" cases (presented in Sec. 4.4.1 in the discussion paper) have been incorporated into the presented inversions from the start of the revised manuscript. These modifications include using the parameters in **Q** derived from RML with the synthetic concentration data (i.e. RML-Inv), incorporating temporal covariance into **Q**, and finally using different model-data mismatch variances by tower. A justification for all of these

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choices is now incorporated into the methods section. Also, in contrast to the discussion paper, the transport error inversions will use RML-Inv parameters derived with simulated transport error.

5. Finally, all metrics of comparison will be presented at the monthly scale, given that longer timescales tend to be of more interest for CO2 fluxes than shorter timescales.

"2) The paper might read more easily if the results of each test were presented along with the description of that test, e.g sec 3.1/3.1.1 followed by sec 4.1, sec 3.1.2 followed by sec 4.2 etc. This allows a reader to only focus on one set of tests at a time, and may mean that some repetition in the text can be removed as readers no longer need to be re-introduced to a topic etc."

The authors agree with this suggestion. The paper will be restructured to focus on three different sets of analyses: 1) using the atmospheric data to estimate covariance parameters (with and without transport error), 2) comparison of flux results from 3 cases with perfect transport, and 3) comparison of flux results from 3 cases with simulated transport error. For each section, the description of the analysis will be presented along with the results of that analysis.

"Specific comments

I think the introduction could be reduced in length e.g. previous work might be described more briefly (especially p22410-22411). Is all the GIM description needed in the introduction since some is covered in the methods section as well? The last paragraph of the introduction also seems to repeat some points that have already been made."

Repetitive parts of the introduction will be removed.

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"Given that the test case is for a relatively short period (1 June to 8 July 2004), it might be good to comment on the feasibility of the method for longer periods in relation to calculating the trajectories (p22416, line 26-28) as well as for the inversion itself."

This paper will be followed by a manuscript describing synthetic and real data results for a 2004 full year inversion. The preliminary results for the full year show that the inversion method is robust over longer periods. Calculating trajectories is also feasible, but very computationally intensive for a full year with a Lagrangian model like STILT. These preliminary results will be alluded to in the discussion /conclusion of the current revised manuscript.

"Perhaps in the final section you might also want to speculate on whether the inversion performance might be expected to be different for winter than summer."

Yes, we expect the inversion performance to be better in winter when there is less variability in both the atmospheric data and the underlying flux field. (This has been confirmed with pseudo-data tests performed for other months, although results are not shown.) This point will be included in the final section of the paper.

"The diurnal variation in the covariance structure of the 3 hour fluxes seems interesting (p22427). Given that the night-time variance is lowest, does this imply that the potential disadvantage of night-time sampling i.e. the smaller footprint, might be offset by the fluxes being representative of a larger area at night? Do you think this would be the case for the 'real world' as well as the CASA model world?"

Yes, if correlation lengths are longer at night, there is a possibility that the smaller footprint of the observations might be offset by the fluxes being representative of a larger area. (The longer correlation lengths at night are also evident with diurnally-varying fluxes from the SiB 3.0 biospheric model, and it seems likely for the true flux field as well, although there is no way to confirm this for the latter.) However, there

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are other concerns associated with using night-time data, particularly for the short towers which are consistently within the night-time PBL. First, given the much smaller footprint at night (in space and time), spatial and temporal aggregation error may be more of a concern. For example, one of the sensitivity tests in the discussion paper with the F8d/C3h case showed much higher RMSE when including night-time data for short towers (p. 22431, lines 2-9). Also, we expect difficulties in the transport models in properly modeling the night-time PBL height when applying the approach with real data. Especially for this latter reason, near-surface night-time measurements are unlikely to be useful for regional inversions in the near future.

"As noted above, the inability to estimate the spatial covariance parameters when random transport error was included seems to be rather a concern (p22427). Would this be worse for non-random transport error (which could easily be the case in the real world)? Do you have any evidence for the suggestion that more data points would improve things - given that with your different temporal aggregations, you have quite a large range in the number of data points that you are currently using? If more data points doesn't help, what other options do you have to estimate these spatial covariance parameters?"

The problem in the discussion paper was specifically with the F8d/C8d case where the sill variance went to zero when random transport error was added to the 45 measurements for this one month. Using 4 months of data marginally helped to improve the results for this case with transport error.

Estimating the spatial covariance parameters with random transport error is no longer a problem in the revised manuscript. The 3 cases in the revised manuscript all use 3-hourly data vectors, and the RML-Inv optimizations with and without transport error produce non-zero sill variances for all cases. With these 3 new cases, we infer a sill variance that is too high and a correlation length that is too low, with the overestimation

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of the sill the worst for the 4-day case, and the best for the 3-hourly case. When random transport error is added to the measurements, the sill variance is reduced, but it actually becomes closer to the "true" value for all cases. Also, in the revised manuscript, we use the RML-inv parameters for each inversion corresponding to the same case, rather than substituting the parameters from one case for use with another case in the inversion, as done in the discussion paper.

We will also stress in the revised paper that the ultimate concern is the impact of the RML-Inv covariance parameters on the estimated fluxes, rather than their correspondence to the "true" parameters from kriging (RML-OK). For example, we show that the biome-scale errors are slightly reduced for the 4-day diurnal cycle case using the parameters from RML-Inv as compared to an inversion using the RML-OK values.

In the future with real data, if inferred spatial covariance parameters were unreasonable, the results from RML-OK with a range of biospheric models could always be used as a substitute method to obtain flux covariance parameters. The impact of non-random transport error remains a concern for all types of inversions, although these are difficult to simulate in a pseudo-data environment. Perhaps systematic transport errors would not reduce the inferred variance of the fluxes as much as random error, and could potentially increase it. All of these points will be clarified in the discussion of the revised manuscript.

"The first paragraphs of sec 4.4 and 4.4.1 seem to say similar things. Try and combine the information. Perhaps the first paragraph of Sec 4.4 should just say that three refinements were tested ... spatial covariance parameter choice, adding temporal flux covariance and allowing model-data mismatch to vary across sites."

As mentioned above, we plan to make these modifications to the covariance matrices at the start of the paper, and these choices will be discussed (without repetition) in the methods section.

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"Figure 9 and associated text (p22434). The text and figure caption says that the mean north american flux is on this figure, but it doesn't seem to be. "

This is true and will be corrected. Thank you.

"These ecoregion results seem rather disappointing - to have only half the region estimates to be within 2 sigma of the true flux would suggest that the flux uncertainties are too small. "

The authors agree that results at the eco-region scale for inversions with simulated transport error in the discussion paper were disappointing. The revised manuscript will show the eco-region scale fluxes from 2 sets of inversions, both with and without transport error. These updated results will demonstrate that we are able to capture the "true" flux within 2 sigma confidence intervals in almost all eco-regions for an inversion without transport error using a case that resolves the diurnal cycle (e.g. 3-hourly or the 4-day diurnal cycle). The revised discussion will then focus on how the quality of the inversion degrades with a (currently) realistic amount of transport error represented as normally-distributed random noise in the measurements. This degradation is particularly acute in the under-constrained areas, as we would expect, given that the random noise added to the measurements overwhelms the diffuse atmospheric signal for these areas. The uncertainties also tend to be too small for these under-constrained areas in an inversion with simulated transport error. The addition of full cross spatial-temporal covariance in the **Q** matrix shows promise in returning wider confidence intervals, but at a greater computational cost and with an additional bias in the inferred fluxes.

The degradation in quality of the inversion results seen in this study with simulated transport error will hopefully improve in the future by using data from a denser measurement network (reducing the areas that are under-constrained by the measurements and magnifying the signal in the well-constrained areas). Also, correcting non-random transport errors that contribute to the high inferred model-data mismatch seen with real

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measurements will help to rectify this situation. Such non-random transport errors may include known systematic offsets in the boundary conditions or problems with the PBL height in the meteorology driving the transport model.

"The sentence (line 22) "However, among the two cases, ..." doesn't seem to agree with the figure. To me, Fd looks closer than F8d to the true flux for the desert region and in the tropics both inversions seem to be more than 2 sigma from the true flux. "

In the desert region (DeXS), the F8d/C3h is closer than the Fd/C3h case to the truth. The F8d/C3h flux is also closer to the truth in the tropics, although the reviewer is correct that both cases do not capture the truth within 2 sigma for this eco-region. The statement in the manuscript was that there was a significant difference between the two cases in these eco-regions (at 1 sigma), not that either was appropriately capturing the true flux within the confidence intervals. However, the authors agree that this may be over-interpreting small differences in the results. With the presentation of the 3 new cases, the discussion of the eco-region fluxes will instead focus on the impact of temporal aggregation error across cases in a perfect transport setup, and the degradation in quality of the inversion (where fluxes tend to revert to the mean) with simulated transport error.

"Figure 9 is the first time that any absolute uncertainty numbers are presented - I wonder whether a root mean square uncertainty would make a good comparison with the RMSEs presented in Fig 5?"

Rather than showing a root mean square uncertainty, we chose to include Table 5 with the % of true grid-scale fluxes within the 95% confidence intervals. Ultimately, these two statistics are giving information about the same thing, i.e. whether the actual errors from the inversion are similar to the predicted ones from the a posteriori uncertainty. This will be clarified in the text of the revised manuscript.

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"p22436, line 9-17: the improvement from using separate model-data mismatches seemed fairly small to me."

The authors agree that a reduction from 0.82 to 0.78 μmol/(m2*s) with the addition of tower-specific model-data mismatch variances for the F8d/C3h case is rather small. However, this reduction is large relative to the range of results for the whole continent with transport error (0.82 to 0.93 μmol/(m2*s). Also, the RMSE is defined at the grid-scale, and therefore, a small reduction in grid-scale RMSE may make more of a difference at larger aggregated spatial scales. Finally, this result was robust across all examined cases, including results not shown in the discussion paper. Therefore, in the revised manuscript, we chose to use tower-specific model-data mismatch values from the start of the paper. This choice may be re-evaluated for future inversions using a larger number of measurement stations.

"p22437, line 1-14: I'm not sure whether this discussion of the Law et al. results is really needed here. The Australian case is more dependent on coastal sites which could behave rather differently to the continental sites that you are reliant on."

Thank you, we will remove this discussion, but still note that an understanding of the impact of non-random transport error remains important for interpreting fluxes from future regional inversions using continental continuous data.

*"**Technical corrections***

p22414, line 4-6. Suggest removing sentence "The naming convention ..."

We think it's important to state the naming convention of the cases in the text. However, this sentence will be rewritten with the 3 new cases.

"p22414, line 7: Suggest adding "(grid-scale)" after 1ox1o"

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Yes, we can add this. Thank you.

“p22414, line 13-14: Suggest removing sentence "For the remainder of this paper .."”

Yes, this makes sense given the previous correction. We will make this change.

“p22416, line 13-14: Remove "which are maintained .... Administration."”

We will remove this.

“p22416, line 19-21: Remove ", or other readily ...noaa.gov)"”

We will remove this.

“p22416, line 28: Suggest adding "these" after "integrating"”

We will add this.

“p22431, line 1: check sec number, need 4.4.1 not 4.3?”

Yes, you are correct. Thank you.

“p22431-22432: check sec numbers - 4.2 should be 4.3? in a couple of places?”

Yes, we will correct this.

“p22432, line 25: add "(0.0 in Table 6)" after negative (if this is true)”

In the revised manuscript, we do not infer any negative transport errors. The negative inferred transport error for the F8d/C3h case in the discussion paper was an artifact of solving for the **Q** and **R** parameters separately.

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"Figure 5: I suggest extending the y axis to 0.00. As plotted, the difference between cases is overemphasised compared to the total error."

Yes, this will be fixed.

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