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Interactive comment on "Investigation of error sources in regional inverse estimates of greenhouse gas emissions in Canada" *by* E. Chan et al.

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General comments: Although I see that the authors have put a considerable amount of work into preparing this study, there are a number of major flaws in the method, which make it unacceptable for publication. First, the influence of land biosphere fluxes of CO_2 is completely ignored. Therefore, this synthetic case study is of no use in understanding the performance of real observation inversions, since real observations are sensitive to land biosphere fluxes. The gross land biosphere fluxes of CO_2 are generally much larger than the fossil fuel fluxes and are the greatest source of uncertainty. By just analyzing an inversion for fossil fuel fluxes, the largest part of the CO_2 inversion

Full Screen / Esc

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Interactive Discussion

Discussion Paper

problem is ignored. Second, there are flaws in the inversion method. The fact that the scalars optimized, λ, apply to the product of the transport and the fluxes, biases in the transport between sub-regions will be folded into the scalars. I have included further details of these problems under "Specific comments". In addition, I am suspicious about the result in the "no flux and no transport error" experiment, in which large posterior errors were found. This should not be the case with no prior and no observation error, which makes me also skeptical about the other results. Lastly, numerous studies have been previously published analyzing transport and other uncertainties on the retrieved fluxes. Unfortunately, this synthetic study fails to bring any new insights in how to best define these uncertainties or set-up the inversion problem.

Authors' response:

The authors would like to thank Referee #1 for the helpful comments. The main objectives of this study are to examine the impacts of errors from the optimisation method, prior flux distribution and the atmospheric transport model, as well as their interactions on inverse flux estimates under a series of controlled experiments. It is not the intentions of the authors to suggest a set-up has been found for real CO2 flux inversions; however the goal is to first identify problems in our inversion set-up before applying it to real observations. This study is useful for regional flux estimations for tracers that have similar temporal and spatial characteristics to fossil fuel CO2 [e.g. wintertime CH4 in Canada with mainly anthropogenic sources (fossil fuel, agriculture and waste or landfill) and essentially no wetland emissions, or possibly in urban areas where the contributions from biospheric CO2 are relatively insignificant], and we will state this clearly in the abstract and the introduction section.

Performing biospheric CO2 flux inversions represent the next level of complexity and would require using prior fluxes with strong diurnal variations and both positive and negative fluxes. It merits a separate study to examine the errors and uncertainties for this case, we plan to examine the different components

of errors for regional biospheric CO2 flux inversion shortly.

It is true as the reviewer noted that 'The fact that the scalars optimized, λ, apply to the product of the transport and the fluxes, biases in the transport between sub-regions will be folded into the scalars.' as in Eqn (1).

$$y_{t,s} = \sum_{p \in R} \lambda_p \sum_{g \in G} M_{g,p,t,s} x_{g,p,t} + \epsilon_{t,s}$$

We follow the usual approach (Gerbig et al., 2003; Lin et al., 2004; Zhao et al., 2009) that it is more reasonable to apply the optimized scaling factors λ_p to the flux in region p only. We assume the transport or meteorological data were already optimized by the model provider (ECMWF) in their data assimilation process and will remain unchanged in our model. The error or biases in the transport is to be accounted for in the error covariance matrix D_ϵ.

The results in the "no flux and no transport error" experiment could be explained as follows. The D_ϵ^{-1} and D_{prior}^{-1} are assumed to be diagonal matrices in Eqns (4) and (5). The erroneous assumption of zeros for the off-diagonal matrix elements would lead to errors in λ (solved from Eqn (5)), including for the "no flux and no transport error" experiment. We plan to evaluate other approximations (with non-zero off-diagonal elements) for the covariance matrices and their impact on the inversion results in future studies.

The resultant errors depend on both the transport and flux distribution [with different covariance error structure depending on the inversion setup (such as region definitions, measurement sites spatial configuration, transport-flux coupling, etc.)]. Our results showed that it needs to be evaluated for each inversion setup, the eastern and western domains in our study showed that results could be very different (depending on transport errors and how the transport is coupled to the flux distribution). Doing inversion without proper

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Full Screen / Esc

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Discussion Paper

assessment of the model could lead to flux estimates with 100% error or greater.

Our view is that it is necessary to evaluate each inversion setup to understand better the inversion model's weaknesses. 'Insights' or 'uncertainty estimates' from other studies can only serve as guidelines in any new inversion. We hope these results or insights will motivate other scientists to carefully test their inversion models as a requisite prior to doing inversion with real observations.

The result in "no flux and no transport error" experiment (E32) for Ontario solving for only 1 sub-region has essentially no error (1%) using the CFM method (and 0% in E1-E10 using MCMC) as shown in Figure 4b. This suggests that there are no problems with the results. The large errors are found when the number of sub-regions (unknowns) is increased. This is reasonable and expected result, because the correlation between sub-regions becomes large which increases the collinearity in this inversion (least-squares linear regression) method.

Mathematically the Eqn (5) that is used to solve for the λ in the CFM method in this study has been shown on page 66 in Tarantola (2005) as the following three equivalent expressions:

$$\boldsymbol{\lambda} = \left(\mathbf{K}^{\mathsf{T}}\mathbf{D}_{\epsilon}^{-1}\mathbf{K} + \mathbf{D}_{prior}^{-1}\right)^{-1}\left(\mathbf{K}^{\mathsf{T}}\mathbf{D}_{\epsilon}^{-1}\mathbf{y} + \mathbf{D}_{prior}^{-1}\boldsymbol{\lambda}_{prior}\right)$$

$$= \boldsymbol{\lambda}_{prior} + \left(\mathbf{K}^{\mathsf{T}}\mathbf{D}_{\epsilon}^{-1}\mathbf{K} + \mathbf{D}_{prior}^{-1}\right)^{-1}\mathbf{K}^{\mathsf{T}}\mathbf{D}_{\epsilon}^{-1}\left(\mathbf{y} - \mathbf{K}\boldsymbol{\lambda}_{prior}\right)$$

$$= \boldsymbol{\lambda}_{prior} + \mathbf{D}_{prior}\mathbf{K}^{\mathsf{T}}\left(\mathbf{K}\mathbf{D}_{prior}\mathbf{K}^{\mathsf{T}} + \mathbf{D}_{\epsilon}\right)^{-1}\left(\mathbf{y} - \mathbf{K}\boldsymbol{\lambda}_{prior}\right)$$

The last expression is in fact identical to for example, Eqn (11) in Thompson and Stohl (2014) as shown below.

$$\mathbf{x} = \mathbf{x}_b + \mathbf{B}\mathbf{H}^{\mathsf{T}}\left(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathsf{T}} + \mathbf{R}\right)^{-1}\left(\mathbf{y} - \mathbf{H}\mathbf{x}_b\right)$$

Specific comments: The abstract is difficult to follow and needs to be improved for clarity (see also comments below).

Authors' response:

We have revised our abstract to include the changes noted by the reviewer as follows.

Inversion models can use atmospheric concentration measurements to estimate surface fluxes. This study is an evaluation of the errors in a regional flux inversion model for different provinces of Canada, Alberta (AB), Saskatchewan (SK) and Ontario (ON). Using fossil fuel CO2 CarbonTracker model results as the target, the synthetic data experiment analyses examined the impacts of the errors from the Bayesian optimisation method, prior flux distribution and the atmospheric transport model, as well as their interactions. The posterior fluxes were estimated by the Markov chain Monte Carlo (MCMC) simulation and cost function minimization (CFM) methods. Experiment results show that the estimation error (or relative percentage difference between the posterior and target fluxes i.e. ((posterior flux - target flux)/target flux)*100%) increases with the number of sub-regions using the CFM method but not for MCMC. For the region definitions that lead to realistic flux estimates on the sub-regional and monthly scale, the numbers of sub-regions for the western region of AB/SK combined and the eastern region of ON are 11 and 4 respectively. The corresponding annual flux estimation errors for the western and eastern regions using the CFM method are 0% and 8% respectively, when there is only prior flux error. The estimation errors increase to 40% and 232%

resulting from transport model error alone. When prior and transport model errors co-exist in the inversions, the estimation errors become 29% and 201%, whereas the estimation errors using MCMC are considerably smaller. This result indicates that flux estimation errors are dominated by the transport model error and different sources of errors can potentially cancel each other and propagate to the flux estimates non-linearly. Although estimation errors can be reduced, increasing the number of sub-regions beyond 11 sub-regions for AB/SK and 4 sub-regions for ON can produce unstable monthly and unrealistic fluxes.

In addition, it is possible for the posterior fluxes to have larger differences than the prior compared to the target fluxes, and the posterior uncertainty estimates could be unrealistically small that do not cover the target. Stable and realistic sub-regional and monthly flux estimates for western region of AB/SK can be obtained, but not for the eastern region of ON. This indicates that it is likely a real observation-based inversion will work for the western region for tracers that are mainly contributed by anthropogenic sources with regional fluxes that have similar temporal and spatial characteristics to fossil fuel CO_2 [e.g. wintertime CH_4 in Canada]. However, improvements are needed with the current inversion setup before real inversion is performed for the eastern region.

P22717, L10: Could the authors please explain what they mean by the "assumed model-observation mismatch", do they rather mean the uncertainty in the observation space? The model-observation mismatch, obviously is just the difference between the modeled concentrations and the observations, which does not need to be "assumed".

Authors' response:

The "assumed model-observation mismatch" is actually the variance of the model-observation mismatch. We assume 30% error for the λ_ϵ similar to other

Full Screen / Esc

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Discussion Paper

studies. For practical reason, the prior variance of this mismatch is assumed instead of estimated. We will clarify this in the text. We have deleted this sentence from the abstract and it will be explained in details in Section 2.8.

P22717, L11: What is meant by "estimation error" do the authors mean the difference between the "target" and posterior fluxes. Please specify.

Authors' response:

The estimation error is the relative percentage difference of the posterior flux and the target flux (estimation error=((posterior flux - target flux)/target flux)*100%).

P22717, L15-20: Please state what these percentages represent - are they the fraction of posterior-target flux difference compared to the target flux? This is unclear. (Note that the abstract should be understandable without having read the entire paper beforehand).

Authors' response:

The estimation error is the relative percentage difference of the posterior flux and the target flux. The percentage definition has been added in the explanation of the estimation error as stated in the previous comment. We will clarify this in the abstract.

P22718, L13-14: It is not true that global inversions are unable to resolve fluxes on smaller than sub-continental scales. A number of inversion frameworks based on global Atmospheric Transport Models (ATMs) with, e.g., use of the adjoint model, re-

solve fluxes on the grid cell level, i.e., order of a couple of degrees. Whether or not these inversions are able to independently constrain the grid cell is a matter of the observation constraint.

Authors' response:

There are global inversions that attempt to resolve fluxes on smaller scales but large uncertainties can be found when one looks into the spatial details. "Whether or not these inversions are able to independently constrain the grid cell is a matter of the observation constraint." True, but other factors such as the inversion model setup can contribute the errors or stability of the inversion results. As shown in this study (as well as other studies showing negative flux inversion results are possible where positive fluxes are expected), the transport model error dominates and unrealistic flux results can be obtained by increasing the number of sub-regions (spatial unknowns) for some inversion configuration (as in ON). Some studies tried to ensure positive definite flux results by assuming non Gaussian error distributions, we will investigate these statistical assumptions in the future.

P22719, L3: There are a number of regional Eulerian models that are used for inversions, e.g. CHIMERE, so please change "typically" to "a number of" or equivalent.

Authors' response:

We have corrected it.

P22719, L4: Generally Lagrangian models are driven by reanalysis data, which are data assimilation products, to say "modeled meteorology" is misleading.

Authors' response:

We have changed it to assimilated meteorology. We actually used analyses and forecasts from the ECMWF model, not reanalysis data.

P22720, L16, By "estimation error" do the authors mean the difference between the posterior and target fluxes. "Estimation error" should be defined.

Authors' response:

The estimation error is the relative percentage difference of the posterior flux and the target flux. We will clarify this in the text.

P22721, L5-6: Is it correct that only the fossil fuel emissions of CO2 were used to simulate CO2 concentrations? If so, were the very large CO2 fluxes from the land biosphere ignored? And if this is the case, then the results of this study are of very limited use (and of no use at all for determining fluxes of CO2), as in order to determine fossil fuel CO2 fluxes, the land biosphere fluxes also need to be determined, and these have the largest uncertainties.

Authors' response:

Please see earlier response to the general comment.

P22721, L22 – P22722, L5: It is well known that having variables that represent large regions (large with respect to the heterogeneity with the region and the influence this has on the observations) is a source of model representation error, or specifically,

aggregation error. This has been shown in numerous previous studies, importantly those of Trampert and Snieder (1996) and Kaminski et al. (2001). The work of Kaminski et al. even provides an algorithm to determine this model representation error in the observation space. On the other hand, while an inversion may not be able to separately constrain the variables at fine resolution, this can be ascertained from the posterior error covariance matrix (seen from negative covariance between variables). In this case, the variables can be aggregated a posteriori to give more robust estimates for the larger regions with smaller uncertainty than for the individual variables since the errors have negative covariance. Therefore, I do not see what can be learned from performing inversion test cases using differing numbers of regions.

Authors' response:

The characteristics of "model representation error (for flux distribution)" (or "aggregation error") and the value (or possible improvement in flux estimation) of "variables can be aggregated a posteriori" are likely functions of each individual inversion setup. In this study, the cases (II) prior flux error, and (IV) prior flux error and transport error, would have "aggregation error"; whereas case (III) transport error only, would not have "aggregation error". Our (MCMC) results showed that case (III) without "aggregation error" have the largest error in the posterior fluxes. While cases (II) and (IV) with "aggregation error" have smaller posterior flux errors (compared to (III) transport error case) and increasing the number of sub-regions (or variables) does not improve the posterior flux estimates significantly. Therefore "aggregation error" does not represent a large error in our results, and it needs to be examined for each inversion setup to estimate its possible impact. The coupling between "aggregation error" and transport error (case IV) could be highly complex and possibly even "offset" each other (note each inversion could be different).

The value of "variables ... aggregated a posteriori" can be seen in it our provincial flux estimates (aggregated a posteriori results). The results can

exhibit large fluctuations in case (III) transport error case, indicating that transport errors cannot generally be reduced by aggregating the a posteriori sub-region fluxes. All our inversion results point to large sensitivity to the inversion model setups and the need to evaluate each inversion setup to characterise the inversion model behaviour to achieve "robust" inversion results. Our case (II) without transport error does yield information on how many sub-regions are needed to reach "robust" results (going beyond to more regions did not yield better flux estimates).

There is still a debate in the community on the best degree of spatial resolution to use in inversions (Peylin et al. 2001; Bocquet 2005). Solving for a large number of regions (unknowns), and assuming them to be independent of each other, leads to undetermined sources (Rivier, 2010). According to Kaminsk and Heimann (2001) published in Science, "The choice of a particular spatial resolution is tightly related to the degree of confidence we attribute to our geochemist's knowledge on spatial heterogeneity of the fluxes and to the transport model that is used...There is probably an optimal number of regions to consider in inverse modeling of CO_2 sources that minimizes both the potential aggregation error and the estimated error." As depicted in Fig. 1 in their comments, the estimation error can increase as the number of sub-regions increases. It is not always straightforward to determine the optimal configuration and the number of regions to be optimized as demonstrated in this study particularly when transport model error exists. The role of aggregation error in this study noted here will be added to the discussion in the manuscript.

P22723, L13: Why was a height of 100m chosen for the surface layer (or using the author's terminology, footprint layer)? If the height was increased, then there is a greater probability of it containing particles and thus, better statistics, on the other

hand, the height of the footprint layer should be within the PBL. What is the influence of changing the footprint layer height?

Authors' response:

We have done sensitivity tests using 100, 200, 300m,..etc. for the footprint calculations. The results have no significant difference. The values of the surface footprint layer are in units of s/(kg/m3). If height was increased, the values would be increased. The footprint values will then be normalized by the increased size of the grid volume that turns out to be the same in units of s/kg when fluxes in units of kg/s are folded. However, this height should be low enough to always be in the boundary layer (e.g., 100 m) but not so low as to have too few particles. Using a rather shallow footprint layer should give more accurate results. For detailed explanations please see Stohl et al. (2003).

P22724, L5: "Cost Function Minimization" (CFM) is very generic, as all Bayeisan methods attempt to find the minimum of some cost function, whether it be using conjugate gradient methods, Newton methods, analytical methods or other. Please specify which method was used here.

Authors' response:

To solve for the cost function, an analytical method was used in this study, or computed according to Eqn. 5 to be more precise. The manuscript revision will include this information.

P22725, L2-4: It is not generally true that the MCMC method requires fewer variables than the method that the authors call CFM. In fact, what the authors call the CFM

method is in principle a least squares method. Eq.1 & 2: The scaling factors should be applied to the fluxes, i.e., the unknown variables, x, and not to the product of Mx. The way that this equation is expressed, one is optimizing the transport as well, which should not be the case, the model M must be assumed to be known within the uncertainties, which are given in the observation space. This means that if transport biases exist between regions, then this will be folded into the scalar estimate.

Fig. 1: related to the above point, I suppose the authors mean by "aggregating the mole fractions to sub-regions" they actually mean the allocation of the transport operator into each of the sub-regions, so that the influence of each sub-region on the mole fractions is separated as shown in Eq. 1?

Eq. 4: Again, the same applies as with the MCMC method, the scaling factors are applied to the product of the transport and fluxes, thus if there are biases in the transport between regions, this is folded into the scaling factors. This is an additional avoidable source of error.

Authors' response:

P22725, L2-4 has been corrected. MCMC does not have a regularization term as in CFM (the second term representing prior flux constraint). Please see earlier response to the general comment. Transport biases among the regions (or errors in general) will be folded into the modelled concentration automatically as long as a transport model is used. But as noted above, the scaling factors are applied only to the fluxes, with the transport unchanged. The CFM in this study is indeed a least-squares method and it has been widely adopted in the community to estimate fluxes by minimizing the difference between observations and model results. CFM is actually originated from Eq. 1&2 when Gaussian and independent residuals are assumed. Please refer to page 64 in Tarantola (2005) for the derivations.

Fig. 1: The simulations were done backward in time and the footprints were

gridded at 0.2x0.2 resolution which allowed us to aggregate into various region configurations. Prior fluxes were folded in the footprints to calculate the modelled concentrations at each 0.2x0.2 grid. The "transport operator" was applied to the FLEXPART output grid level. Thus "aggregating the mole fractions to sub-regions" is similar to "the allocation of the transport operator into each of the sub-regions". We modified the text: "aggregating the mole fractions to sub-regions (or the allocation of the transport operator into each of the sub-regions)" to make it clearer.

Eq. 4: Since the constraining data in this study are concentrations or mole fractions (and not fluxes) acting on modelled concentrations (with the transport folded into the prior fluxes), transport biases among the regions are represented or approximated in the error covariance matrix $\mathbf{D}_c$.

P22728, L9: While it is true that the real error covariances are not known, it is not true that the prior error covariance matrix, $\mathbf{D}_{prior}$, is typically assumed to be diagonal. A lot of research has been done (and papers published) on defining patterns of error covariance in these matrices.

Authors' response:

We have corrected this statement.

P22730, L3-5: Because the main fossil fuel sources, e.g., industry, transport, power plants etc. remain largely the same between two consecutive years there will be a strong correlation between the CT2010 and CT2011 fluxes. Therefore, the inversions for the "flux error case" do not represent the reality in which the flux error may have a very complicated structure.

Authors' response:

We intended to demonstrate the problems with inversions even with such small flux error. Therefore, one can expect much larger flux estimation error in reality. We will clarify this in the revision.

P22730, L20-21: These synthetic experiments do not account for the land biosphere fluxes of CO_2, which strongly influence real CO_2 observations. The co-dependence of transport errors and CO_2 land biosphere fluxes is a very important source of error in CO_2 inversions, e.g. the seasonal and diurnal so-called "rectifier" effects. By ignoring these, this study is of limited use to real observation inversions of CO_2.

Authors' response:

We apologize for the confusion. We did not mean to imply that the inversion method could work for real CO_2. We will clarify this in the abstract and in the introduction section. As noted previously, the results of this study are useful for flux inversion with similar spatial and temporal prior fluxes (e.g. wintertime CH_4 in Canada with mostly anthropogenic emissions, or in urban areas where the contributions from biospheric CO_2 are relatively insignificant). This study is meant to demonstrate using small flux and transport errors depending on the region definitions (or number of sub-regions) that the estimation errors can already be very large.

P22734, L18: The fact that the posterior error is considerable in the "no prior flux error and no transport error" case makes me suspect that there is a bug in the set-up.

The modeled – pseudo-observation differences must be zero, thus the optimal fluxes should be very close to the prior fluxes, which in this case is also the target fluxes.

Authors' response:

As noted in the general comments, the results in the "no flux and no transport error" experiment could be explained as follows. The D_ϵ^{-1} and D_{prior}^{-1} are assumed to be diagonal matrices in Eqn (4). The erroneous assumption of zeros for the off-diagonal matrix elements would lead to errors in λ (solved from Eqn (5)), including for the "no flux and no transport error" experiment. We plan to evaluate other approximations (with non-zero off-diagonal elements) for the covariance matrices and their impact on the inversion results in future studies.

The resultant errors depend on both the transport and flux distribution [with different covariance error structure depending on the inversion setup (such as region definitions, measurement sites spatial configuration, transport-flux coupling, etc.)]. Our results showed that it needs to be evaluated for each inversion setup, the eastern and western domains in our study showed that results could be very different (depending on transport errors and how the transport is coupled to the flux distribution). Doing inversion without proper assessment of the model could lead to flux estimates with 100% error or greater.

P22743, L15: I think it is pure coincidence that there is a cancelling effect between the flux and transport errors. This is generally not the case.

Authors' response:

We will revise this statement. There could potentially be cancelling effect (or compensating errors) in reality but it would be difficult to determine when real

Full Screen / Esc

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Discussion Paper

observations were used.

Technical comments English language editing is needed especially in the use of articles and punctuation. I have pointed-out only a few examples here:

P22717, L22: "having" should be "to have P22717, L23-24: words missing in "could be unrealistically small that do not cover the target"

Authors' response: Corrected.

P22718, L2: missing article "a real inversion"

Authors' response: Corrected.

P22718, L8: please change to "in the context of national reporting of emissions"

Authors' response: Corrected.

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Interactive Discussion

Discussion Paper

P22718, L12: punctuation "Global inversion systems, such as CarbonTracker, which ..."

Authors' response: Corrected.

P22718, L14: "at subcontinental scales"

Authors' response: Corrected.

P22719, L8: change "annual" to "1-year" as "annual" is an adjective

Authors' response: Corrected.

P22719, L11: "...apply to..."

Authors' response: Corrected.

P22720, L25 – P22721, L4: This sentence is very long and difficult to understand. After reading it twice I realized that adding the correct punctuation helps: "...atmospheric inversion, using simulations run in a backward (adjoint) mode, are: the synthetic..." but please consider revising.

Authors' response: Corrected.

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Full Screen / Esc

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Interactive Discussion

Discussion Paper

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