Geoscientific
Model Development
Discussions

Interactive comment on "Weak-constraint inverse modeling using HYSPLIT Lagrangian dispersion model and Cross Appalachian Tracer Experiment (CAPTEX) observations – Effect of including model uncertainties on source term estimation" *by* Tianfeng Chai et al.

Tianfeng Chai et al.

tianfeng.chai@noaa.gov

Received and published: 4 October 2018

This study investigates the performance of a source term estimation method using data from the CAPTEX controlled release experiment. The interest in this experiment is that the source strength is known, as in OSSE's. However, unlike theoretical OSSE experiments real data are used, which allows assessing the role of transport model uncertainties and how to account for them. In principle this is all very interesting,

however, the outcome remains on a very technical level. It is not clear what we learn here that was not known already. There is little justification of the error assumptions that are used. In OSSE's this is fine as long as the world is self-consistent (or deliberately not), however, the use of real data calls for a justification of what is assumed. Almost no attempt is made to test whether the statistics are self-consistent (e.g. chi-squares, biased residuals, etc.). Hardly any effort is made to interpret the results: how to explain them, and to what extent are they within expectation. Furthermore, no attempt is made to relate the outcome to what was done before. These aspects will need further effort to make this manuscript suitable for publication.

We thank the reviewer for reading the manuscript thoroughly and providing the insightful comments and constructive suggestions.

Using data from the CAPTEX controlled release experiment, it provides a unique opportunity to evaluate the source term estimation more realistically than OSSEs. In the literature of parametric estimation problems, the model uncertainties are given as static terms and they will not vary with model source terms. We try to emphasize this by adding "the effect of including model uncertainties on source term estimation", as a subtitle.

In abstract, "Before introducing model uncertainty terms" has been changed to "Before introducing model uncertainty terms that depend on source estimates".

For simplification, both observation and model errors are assumed to take the linear form and uncorrelated. This can certainly be improved in the future, they seem to be adequate to demonstrate the benefit of using the model uncertainty terms that depend on source estimates.

The self-consistency of the method has been checked. Probability density functions of $ln(c^h) - ln(c^o)$ for the six CAPTEX releases using the estimated source terms are added as Figure 5. The following paragraph is also added in Section 3.5 to justify the normal distribution assumption of $ln(c^h) - ln(c^o)$ and interpret the results.

An assumption made in this inverse modeling algorithm is that the differences between model and observation have a normal distribution with a zero mean. Figure 5 shows the probability density function (pdf) of $ln(c^h) - ln(c^o)$ for the six CAPTEX releases using the estimated release rate q' listed in Table 12. The pdf distribution of $ln(c^h) - ln(c^o)$ for Release 2 is consistent with the normal distribution assumption, and the pdf for Release 4 shows the largest deviation from a normal distribution, while those for the other four releases resembles normal distribution to some extent. The largest relative error for Release 1 is likely related to the negative mean of the $ln(c^h) - ln(c^o)$ distribution shown in Figure 5. The overestimated q' probably results from the compensation of the model bias. Note that the better performance using $ln(c^h) - ln(c^o)$ than $c^h - c^o$ is believed to be caused by the fact that normal distribution assumption is mostly valid for the former but probably invalid for the latter.

In addition, the expected error $\epsilon_{q'}$ of the estimated release rate when assuming the actual release location is known has been calculated for each release. They are listed as the last column in Table 12. The following text has been added to the fourth paragraph in Section 3.5.

The posterior uncertainties of the release rate estimates $\epsilon_{q'}$ are also calculated and listed. They range from 1.8 kg/hr for release 2 to 6.2 kg/hr for release 1. The apparent underestimation is likely due to the model uncertainty assumption, including its simplified formulation as well as the chosen parameter values.

To highlight the difference between this work and what was done before, the following sentence is added to the Summary section besides the change made in Abstract.

Unlike other STE applications where model uncertainties are either ignored or assumed static, we introduce the model uncertainty terms that depend on the source term estimates.

Specific comments:

- *Abstract, line 12, 13: To me it seems that if the problem is linear, averaging outcomes of inversions using different models should lead to the same result as using the average model for in a single inversion. Differences are then due to non-linearity (e.g. using a logarithmic cost function)*

  We agree with the reviewer's statement on the linear systems. As the referee pointed out, logarithmic cost function will result in non-linearity. For the current inverse system that minimizes the cost function with a background term, the average of inversion results using two different models are not identical to the inversion results of using the average of the two model TCMs even without logarithmic concentration differences in the cost function.

- *Page 5, equation 1: The smoothing part of the cost function is included but not used. In that case just leave it out.*

  We removed the smoothing term from both Equations 1 and 5.

- *Page 10, section 3: The explanation of how you normalize the cost function comes only at the end. To follow the discussion preceding that point it would be clearer to move it to the beginning of the section.*

  Following this suggestion, we moved Equation 5 and the rewritten preceding text shown below to the beginning of the section before introducing Figure 3.

  To avoid having zero source as a global minimizer in such situations, the sum of the weights of the mismatch between model simulation and observations is kept unchanged for varying q_{ij} by normalizing it with the weight sum when $q_{ij} = q_{ij}^b$, as shown in Equation 5.

- *Table 10, 11, 12: What is missing here is an estimate of the posterior uncertainty. Otherwise there is no references to compare the actual performance to the expected performance. Without this information it is difficult to judge how important*

model uncertainties are. Of course, the outcome will depend on the assumed flux and observational uncertainties. However, some discussion of the validity of the assumptions regarding those is needed anyway.

The posterior uncertainty, $\epsilon_{q'}$, has been calculated for each release and they are listed as the last column in Table 12. The following discussion has been added to the fourth paragraph in Section 3.5.

The posterior uncertainties of the release rate estimates $\epsilon_{q'}$ are also calculated and listed. They range from 1.8 kg/hr for release 2 to 6.2 kg/hr for release 1. The apparent underestimation is likely due to the model uncertainty assumption, including its simplified formulation as well as the chosen parameter values.

- *Page 17, line 14-15: How significant is the finding of logarithmic inversions giving better results? Looking at your results it seems to me that they may largely be explained by a few high measurements that the model cannot really resolve at the resolution that is used. The logarithmic cost function may allow more flexibility to cope with a few "outlines". This could also explain the dependence of your results on relative observational error. Would this conclusion be different if you filter for data that the inversion has difficulty reproducing.*

This finding of logarithmic inversions giving better results is not new. Chai et al. (2015) has more discussion on the choice of both control variables and metric variables using "twin experiment" settings. Figure 2 shows that there are no apparent "outlines" when the exact release terms are applied in the HYSPLIT simulation. We believe that the reason the logarithmic inversion works better is due to the large range of the concentrations and the log-normal distribution of the concentration differences between model predictions and observations. The newly added Figure 5 and associated paragraph mentioned earlier have more explanation on this.

Chai, T., Draxler, R., and Stein, A.: Source term estimation using air concen-

C5

tration measurements and a Lagrangian dispersion model - Experiments with pseudo and real cesium-137 observations from the Fukushima nuclear accident, Atmos. Environ., 106, 241–251, 2015.