Response to reviewer RC2

The following is my reply to RC2, whose comments are reproduced in italics. Anticipated actions for the revision are also highlighted.

In this study, the author has developed a simple flux inversion analysis tool, named as EnviFlux, for estimating surface fluxes of atmospheric constituents. It is no doubt that this kind of tool is useful, because a flux inversion tool that is used practically for inverse analysis is computationally expensive. It is sometimes difficult to use a practically used system for several sensitivity studies, though those sensitivity experiments are needed to evaluate reliability of inversion results. I have found this simple "toy model" scientifically sound, however I cannot recommend this manuscript for publication because of two major reasons described below.

Many thanks to the reviewer for their time and effort in providing valuable feedback. I am pleased that the reviewer has described this model as "scientifically sound". I am very surprised in their belief that the paper should not be published, and on their assignment of some lower scores, and their belief that the work is not novel. I think these are harsh opinions which I disagree with, and I hope The Editor will read my detailed replies and decide to proceed with paper revisions. The reviewer has, however, raised some interesting issues and I can defend the work against their comments with some modifications to the manuscript. I will be as concise as possible.

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1. No information of computational efficiency or useful facility as a tool

Given the information described in this manuscript, this model seems not to have any advantage other than simplicity compared to other existing models (e.g., lacking turbulent and cloud convection processes, not assuring tracer masses). However, the most important things, how simple and easy to use as a tool this model is, are not well described. How fast this model can run should be explicitly discussed compared with existing models. I do not think just using the semi-Lagrangian scheme cannot make the model faster than others as this technique is often used in existing models. In addition, not implementing turbulent or cumulus convection scheme may make the model fast, but it does not provide novelty of the study, because other models can do the same thing by just turning off those processes.

The paper concentrates on the scientific set-up of the model and inverse method, with some demonstrations, I can provide information on run time, memory, etc (see e.g. my response to Reviewer 1). I am not aware of any other such inverse model that can be run on a low-spec computer, such as a basic laptop, as other such systems rely on high-performance computing infrastructure. My implementation of the semi-Lagrangian method is especially efficient as after it has run once, it stores the trajectories' departure points, making it extremely fast thereafter. This is especially advantageous as the model and adjoint are run many times. I am not aware that other models do this. I can document this (and the resources needed to run the system) in the revision. Turbulence and convection parametrisations can be added in a future development, but the emphasis here is on studying the limitations of inverse modelling per se, which can be done most simply without these processes at this stage.

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2. Too simple experimental design

Usually, during development of this kind of inversion analysis model, one should perform ideal experiments to see whether the model appropriately works or not. In that sense, the experiments the author showed in this manuscript are not novel.

I do not agree that experiments are not novel. I believe, in particular, that the experiments demonstrating the ability of the 3D inverse model to identify the positions and strengths of the a-priori unknown source and sink, are novel. In addition, the work shows the consequences of having observation biases and model error. I am not aware such experiments have been done before (the reviewer has not provided any citations to support their claim that the work is not novel).

Furthermore, scaling vertical wind speeds, the author applied to see the effects of model errors, is too simplistic and the results may not provide scientifically useful information. If the atmosphere is considered as hydrostatic (this assumption is usually valid), horizontal wind velocities should accordingly be corrected when vertical velocity is changed. Just changing vertical velocities would deteriorate the consistency with the continuity equation and induce considerable errors in mass conservation. It means that unexpected sources or sinks would occur in the atmosphere, which is not suitable for simulations of long-lived species such as CH_4.

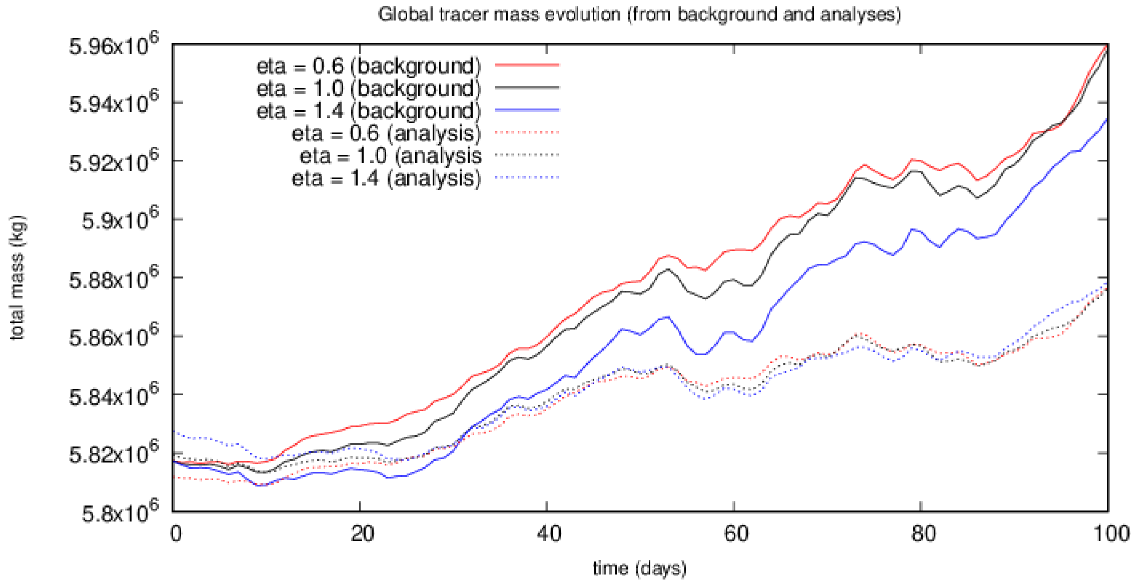

Figure 1: Total tracer amounts for backgrounds (solid) and analyses (dotted) with three different η values: 0.6, 1.0, and 1.4. The factor η multiplies the vertical winds in each respective assimilation/forecast experiment.

The vertical wind scaling $w \to \eta w$, $\eta \sim \mathcal{O}(1)$ is meant to be a simple way of adding model error. It is true that scaling only the vertical wind will lead to extra sources and sinks appearing, which would have the form

$$\rho w(1-\eta)\frac{\partial \chi}{\partial z},$$

where ρ is the air density (not affected by η being different from unity, see below), χ is the tracer mixing ratio, and z vertical distance. Indeed, the whole point of these experiments is to ask how the system compensates for such model error. (Anomalous sources and sinks can result from erroneous use of convective parametrisation in systems where that is applied, so this set-up is relevant.)

One can see the compensating effect in Fig. 1 here. The solid lines are the evolutions of global mass of tracer with three different values of η (see the caption), each based on the same background (a-priori) state (made up of initial conditions and surface fluxes). The values are quite different between the runs, showing the effect of the erroneous sources. The dotted lines are based on the respective analyses, each found by assimilating the same total column observations. Each analysis integration converges in time to similar total tracer masses even though each has a different realisation of model error. The source and sink distributions are different in each integration to compensate for the model error. This is a fundamental issue in inverse modelling, which EnviFlux can be used to investigate further (ideas are given in Sect. 6 of the manuscript).

In terms of mass conservation and hydrostatic balance, the consequences of $\eta \neq 1$ are not as profound as the reviewer states as the vertical wind scaling is applied only to the tracer transport and not to the air mass constituting ρ. The analogy in NWP for instance would be to solve the main prognostic equations (including for the air density) using w, but advecting the tracer with ηw. The anomalous sources and sinks of the tracer would have negligible effect on hydrostatic balance since the tracer has negligible mass contribution.

The above points can be discussed in the paper revision and will add to the quality of the paper.

In addition, the author did not consider atmospheric sink of CH4 due to oxidation with OH, which is one of the most important features of atmospheric CH4.

The paper is not meant to be an analysis of methane, but instead a methane-like tracer (having similar patterns of sources and sinks in the latter part of the paper, but no methane oxidation with hydroxyl radical) so that the inverse problem can be studied in its simplest form. I will emphasise this in the revision.

Minor comments:

1. *L25-26: CO2, CH4, N2O; because they appear first, they should be fully spelled-out.*
2. *L34: That is true also for 4D-Var here.*
3. *L42: That is true also for CO here.*
4. *L76: Please specify what χ is here (e.g., mass concentration, mole fraction, mixing ratio).*
5. *L77: Please elaborate how to derive wind velocities and diffusion coefficients. Are they taken from reanalysis data?*
6. *L78: "u = (u v w)" should be a transpose of a vector, i.e. "u = (u v w)T"*
7. *L82: "ppb" should be explained as "parts per billion". In addition, this is not usually used as the unit of mixing ratio, but as that of dry air mole fraction.*
8. *L86: What does "τρ" mean?*
9. *L110: "For the experiments shown in this paper, no explicit diffusion is applied" This is a critical flaw of the experiments, which makes the results unsound.*
10. *L117: "EnviFlux does not include (sub-grid) turbulent or convective transport process" I think that if a model does not include these processes, it cannot appropriately simulate any atmospheric constituent transport. This flaw critically affects its inversion results.*
11. *L165: Does "total column amount (TCA)" mean vertically integrated amount? Usually, satellite products provide column averaged amount.*
12. *L169: "The TCA observations are found from a discretization of . . . " The author should note that satellite data are made with averaging kernels, which should also be incorporated in the model.*
13. *Table 1: Please elaborate the experimental settings of Table 1 in detail in the main text. Please explain the validity of experimental length of 100 days and source time-step of 30 days (while temporal correlation scale is 3 months, I'm wondering if these settings are reasonable). "nx = 33, ny=65" looks strange to me, because the number of longitudes is usually larger than that of latitude. Furthermore, how long the assimilation window was set should be clarified. Please explain the validity of the number of 4D-Var iterations (=25). Is it enough to converge the parameters?*
14. *L256-257: "Here, each is taken as a point location in the horizontal. . . " Is the satellite orbit assumed here derived from GOSAT? Are data gaps due to clouds (typically existing in the tropics) considered?*
15. *L443: "a simplified tool" From my point of view, the model looks unmatured rather than simple. If the author claims this simplicity is advantageous, that should be elaborated.*
16. *L446: "cheaply without the need for high performance computing" To claim this, the author should describe what kind of machine was used and specify wall-clock time for each experiment. Furthermore, the author should also demonstrate those computational utilities by comparing with other existing models.*

The above minor points can be addressed in the revision. Comments on some of the points that may require response now are as follows.

- Point 9: diffusion is often added to stabilise a numerical advection scheme. The semi-Lagrangian scheme however is stable, and so explicit diffusion is not found to be needed to produce meaningful evolution. Semi-Lagrangian schemes introduce some numerical diffusion, so in effect, diffusive processes are present.
- Point 10: this version of the model is a toy model and was developed to study the inverse problem rather than to simulate an actual real-world tracer. The purpose of the system is to strip-down the problem into its fundamentals in order study the limitations of inverse problems, and in later work to propose and test solutions. This is a valid approach for these purposes and is often done in mathematical physics.

I hope I have helped argue that the system is a useful tool and that the paper is a valid scientific study, and with revisions, would make an interesting contribution to GMD.