

Responses and revisions to reviewers after revision 2 for: 2025-6352, EnviFlux (v1.0): a simplified surface flux inversion tool based on four-dimensional variational data assimilation (4D-Var)

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This document is a summary of the Reviewers' comments, my replies, and descriptions of my revisions.

Responses and revisions for Reviewer 1

The following is a copy of Reviewer 1's comments in italic. My responses are in Roman font. Many thanks to Reviewer 1 for their time and effort in checking my revisions.

I am satisfied by the authors' response to my comments, and in particular the more detailed discussion of computational performance has helpfully illustrated EnviFlux's potential role in flux inversion experimental design. I recommend publication as-is.

Thank you.

Responses and revisions for Reviewer 3

The following is a copy of Reviewer 3's comments in italic. My responses are in Roman and action points to produce revision 3 of the manuscript are in blue. Many thanks to Reviewer 3 for their time and effort in reading my revised paper, and for the insightful comments.

1. The model-error experiment perturbs only the vertical wind component while assuming the horizontal winds are perfectly known. Please clarify the rationale for excluding horizontal wind errors, which can be an important source of transport uncertainty, and discuss whether the conclusions are expected to extend to horizontal wind/transport errors.

While the vertical winds are scaled, the horizontal winds are not perturbed to maintain broadly the right amount of lateral transport to allow the tracer to circulate globally with broadly the correct extent. If the horizontal winds were scaled with the same factor as the vertical winds, the tracer would either be more constrained locally ($\eta < 1$) or be transported horizontally too quickly ($\eta > 1$).

Actions: Added text to start of Appendix G (which was Appendix F in the reviewed version of the manuscript), the start of Sect. 4.2, and the second paragraph of Sect. 6.1.

2. The manuscript appears to treat the tracer as chemically inert and does not include methane chemical loss. Please clarify this assumption and discuss its implications for applying EnviFlux to methane inversions, particularly for longer transport times and global/regional domains where chemical loss may become non-negligible.

The paper is based on a hypothetical tracer that is subject to surface source/sinks (in a similar way to methane in the second application), but with no chemical processes. This is a reasonable approximation given that the system is intended to be a low-cost tool to help understand fundamental elements of inverse problems, rather than to be a model for direct comparison with the real world. Some suggested further investigations are given in Sect. 6.2. The resolution (including the number of vertical levels) could be reduced to make the system even lower cost. Stripping down a problem to its essentials is a common approach in science, especially in data assimilation where simplified models are used to test new ideas (e.g. use of the suite of Lorenz models [14, 4, 6, 13], shallow water equations [2, 7, 9, 11], and even three-body gravitation models to study different timescales in physical systems [8]). There seems to be a gap in the literature where simplified models are available to look at the inverse transport problem, and hopefully EnviFlux can help to fill that gap as there is still much to learn about inverse problems, even though they are routinely used.

Adding chemical loss and production would add cost, complexity, and potentially non-linearity. The problem would no longer be a pure transport inverse problem and parcel trajectories would be subject to modification of the mixing ratio, potentially dependent on sunlight, cloud cover, temperature, and concentration of other constituents. Should the chemical modification be incorrect, and where the process is observed (directly or downstream), I would expect the upstream surface fluxes to be erroneously modified to compensate. My argument is that a deeper understanding of inverse problems (rather than just applying them) needs to start with the basics.

Actions: Text is added to Sect. 6.1 and 6.2 to clarify the simplicity of EnviFlux. Brief discussion of implications of adding chemistry is included in the second paragraph of Sect. 6.2.

3. The manuscript refers to the vertical density weighting used to construct TCA as an "averaging kernel." This is potentially misleading because it is not equivalent to the averaging kernel of an actual satellite retrieval. Please clarify the distinction and better qualify the representation of satellite observations.

Apologies, I meant that it has the same mathematical structure as a Jacobian.

Actions: Changed text in Sect. 3.2.

4. The manuscript states that 20 iterations are sufficient for convergence, but convergence diagnostics are not shown. Please provide a representative cost-function or gradient-norm convergence plot to demonstrate that the reported results are not affected by incomplete minimization.

Actions: Corrected to 25 iterations, and added a new Appendix (F) showing how J reduces with 4D-Var loop number, referenced from near the start of Sect. 4.

5. Line 533: Authors have provided citations of relevant studies for some of the questions but not for all of them. Here are some relevant studies that might be included:

- Magallanes-Quintanar, R., Galván-Tejada, C. E., Galván-Tejada, J. I., Gamboa-Rosales, H., Méndez-Gallegos, S. D. J., & García-Domínguez, A. (2024). Neural hierarchical interpolation for standardized precipitation index forecasting. *Atmosphere*, 15(8), 912.
- Machine learning emulator: Dadheech, N., & Turner, A. J. (2026). Simulating out-of-sample atmospheric transport to enable flux inversions. *Atmospheric Chemistry and Physics*, 26(1), 427-441.
- Land surface parameterization: Zhang, H., Hendricks Franssen, H. J., Han, X., Vrugt, J. A., & Vereecken, H. (2017). State and parameter estimation of two land surface models using the ensemble Kalman filter and the particle filter. *Hydrology and Earth System Sciences*, 21(9), 4927-4958.

Actions: These are very helpful. Added [3], [15], and some other references ([12, 10, 1]).

Responses and revisions for Reviewer 4

The following is a copy of Reviewer 4's comments in italic. My responses are in Roman and action points to produce revision 3 of the manuscript are in blue. Many thanks to Reviewer 4 for their time and effort in reading my revised paper, and for the insightful comments.

The author applies expertise in the variational assimilation system design developed in weather forecast field to a stable tracer flux inversion using a toy transport model. Although the toy model is impractical for long lived tracers as it doesn't have important physical processes and no mass conservation, the assimilation code provided by author on separate repository can be combined with a mature transport model and adjoint for applications in GHG inversions. Compared to other variational models this one is relatively well documented and accessible. The current version is revised in response to reviews. Recommend publishing with technical corrections.

Many thanks.

As for assimilation system design, it would be useful to note the impact of the original techniques by Fisher and Courtier, 1995 that are behind early studies like Meirink et al. 2008.

Actions: Added [5] to near the end of Sect. 6.2.

L85 The species of interest for this system, could be stable tracers like CO₂ or SF₆. Those concentrations are reported in mol/(mol of dry air). Even if the choice of units is mkg/kg which is not critical given the constant air density, better to remind the user the units in actual application should be per dry air mass.

Actions: Text added in paragraph after Eq. (1).

References

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