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Interactive comment on "FLEXINVERT: an atmospheric Bayesian inversion framework for determining surface fluxes of trace species using an optimized grid" *by* R. L. Thompson and A. Stohl

Anonymous Referee #1

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This paper outlines the development of an inverse modelling software package "FLEXINVERT". The methods employed have mostly been published elsewhere and are well known. Therefore, whilst there are relatively few new insights in this article, the paper is a very thorough and clear account of FLEXINVERT system. I think it will be suitable for publication in GMD, once the following comments have been addressed.

General comments

One of the main findings in the paper is how sensitive certain parts of the inversion are to "background" mixing ratios. This is well known for Lagrangian model inversions, but I think it merits further discussion here. In this paper, baselines are either estimated

using an Eulerian model, or from the mole fractions directly. There are number of problems that occur to me: a) In the case that optimized TM5 mole fractions were used, there is an element of circularity, because the TM5 mole fractions will have already seen the observations. b) In the case where the lower quartile of observations were used, did the authors take into account the fact that the lowest measured mole fractions can have a wide range of origins? In particular, for methane, when air enters Europe from the Southerly sector, it can be significantly depleted in methane, compared to other "baselines" from the Atlantic? If I understand their method correctly, the baselines they obtain would be rather smoothed, and would not identify short-timescale "low methane" events. Even more significant "depletions" have been observed elsewhere in the world, for example in East Asia, where the air can rapidly fluctuate between Northern and Southern hemispheric during the summer. c) In the case where these baseline mole fractions were optimized, there is also an element of circularity, as the observations themselves have been used to determine the "prior". In each of these cases, there is the potential for the choice of baseline to erroneously influence the derived emissions either through biases (that would likely not be well accounted for in the uncertainty quantification method outlined, which assumes only stochastic errors). I don't think the paper needs to solve these problems. However, I think the discussion could be expanded very slightly to further highlight some limitations.

Specific comments

Page 3754, line 13: I'm not sure what this sentence means, or whether "smearing" is the best word to use.

Page 3761, line 11 and Equation 6: I'm not entirely clear why this is necessarily an aggregation error. I think you can formulate this problem so that y_mod for the variable grid is identical to that obtained using the full grid, by using the emissions-weighted footprint. In that case, the aggregation error would only come in during the inversion.

Equation 7: I think F_out should be lower case

Page 3762, Line 26: I think this should be a numeric “1”, rather than “one”

Page 3766, Line 18: This idea has been used elsewhere. Perhaps a reference or two should be given.

Page 3768, Line 2: superscript “T” for transpose in the line below the equation.

Section 2.9: If I read this correctly, it appears that this “non-negativity” correction only applies to those grid cells where negative emissions were obtained? I reality, if the first inversion could “see” this constraint, wouldn’t its effects be felt further away than the individual grid cells where negative emissions were derived? Perhaps a line or two of clarification, could be provided.

Page 3768, Line 26: Appendix C

Page 3770, Line 22: What about the representation error at the flask sampling sites?

Page 3774, Line 24: This assertion could be tested by running the model at a higher release height.

Interactive comment on Geosci. Model Dev. Discuss., 7, 3751, 2014.