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# ***Interactive comment on “Comparison of ensemble Kalman filter and variational approaches for CO<sub>2</sub> data assimilation” by A. Chatterjee and A. M. Michalak***

## **Anonymous Referee #1**

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### **1 Introduction**

The authors compare the performance of two algorithms for CO<sub>2</sub> atmospheric inversion, an ensemble filter and a variational scheme, on a toy problem. The paper has been designed to guide the usage of each algorithm class and to show possible directions for future developments. This ambitious topic is rather fairly covered by the authors, but they have simplified one of the algorithms in a way that significantly reduces the prospect of the paper. There are also some weak paragraphs. I therefore recommend publication provided the following comments are properly addressed.

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## 2 Major comment

For CO<sub>2</sub> atmospheric inversion, the main advantage of 4D-VAR is the capability to address very large inversion problems, and in particular to process large inversion windows seamlessly, respecting both the physics (mass conservation) and the statistics (the prior/posterior uncertainty about each state variable is rigorously propagated forward) throughout the period of interest.

In this context, it is very surprising that the authors make use of overlapping windows (p. 12850, l. 6, actually without any information given about the window length). The reason given in p. 12848, l. 20 (computational cost associated with calculating the inverse of the prior error covariance matrix), does not hold: the computational cost of the transport model in the 4D-VAR inversion makes the cost of the matrix operations negligible (see, e.g., Le Quéré et al. 2007 or Chevallier et al. 2010 for the application and Yadav and Michalak 2012 for the principles). Note that the existence of temporally-correlated prior errors stated in l. 22 (same page) does not favour splitting the inversion problem into small windows.

For this reason (and, to a smaller extent, for those given in my first two minor comments), the particular 4D-VAR algorithm used here should not be called “state of the art” (p. 12828, l.24), but in that case the paper loses much of its appeal. The algorithm should be upgraded for the final version.

## 3 Minor comments

- In p. 12840, the text discusses preconditioning for 4D-VAR and restricts it to “very specific assumptions of the correlation structure and sparsity”. I was actually not aware of 4D-VAR applications without preconditioning. Further, I would argue that such “specific” assumptions are more relaxed for 4D-VAR, that can access

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- both small and high spatial resolutions in the state vector and both short and long inversion windows (with long temporal correlations), than for EnSRF, that has to be run at coarse resolution and with short windows.
- Little is written about the two algorithms themselves. For instance, from p. 12848, l. 10, the reader may guess that the minimiser of the 4D-VAR is L-BFGS. Actually, if this guess is correct, it is not the best choice and would explain why the authors need so many iterations: the Lanczos algorithm (e.g., Desroziers and Berre 2012, and references therein) converges much faster for linear problems.
  - The text repeatedly considers the absence of second order statistical moments in output of 4D-VAR as a weakness compared to EnSRF (p. 12838, p. 12839, p. 12845, p. 12849). Indeed the raw algorithm does not provide an error covariance matrix directly. In p. 12849, l. 22, the text mentions that solutions exists but are ‘extremely expensive’. However, such solutions are routinely used and have formed the basis of many papers (e.g., Chevallier et al. 2007, 2013). The existence of these papers demonstrates that such methods are not ‘extremely expensive’. It can also be shown that these approaches can fasten convergence of the reference inversion (Desroziers and Berre 2012). In other words, the second order statistical moments can be obtained from 4D-VAR if they are needed, even though it is more (only more) expensive. On the EnSRF side, the paper emphasises its capability to produce these quantities, but without studying the quality of these products. These two points bias the discussion and invalidate the conclusion given in p. 12845 (“the ENSRF is more desirable for attribution purposes, wherein source/sink estimates with confidence bounds can be used to gain better. . .”).
  - In p. 12841, operational constraints are simulated by reducing the ensemble size to 100, given a domain of 300 pixels. In proportion, this is still much larger than the ensemble systems quoted in the introduction and therefore dramatically

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- damps the performance loss. Tests with a smaller number (e.g., 10) should be shown.
- In p. 12842, l. 11, the authors suggest using a dynamical flux model. This is a fait point, but the discussion should state that this is already achieved in CCDASs (e.g., Rayner 2010) at the cost of adding significant model errors (e.g., Kuppel et al. 2013), therefore reducing the performance of the inversion in terms of inverted fluxes.
  - p. 12827, l. 13 and elsewhere: the exclusion of batch schemes from the DA group is not appropriate since batch schemes should yield the same solution than the “DA” schemes if perfectly implemented.
  - P. 12849, l.7: It is not clear why the study by Gejadze et al. (2012) is referenced in this context, since it applies to very non-linear systems.

### References specific to this review

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Rayner, P. J.: The current state of carbon-cycle data assimilation, *Current Opinion in Environmental Sustainability*, 2, 289–296, doi:10.1016/j.cosust.2010.05.005, 2010.

Yadav, V. and Michalak, A. M.: Technical Note: Improving computational efficiency in large linear inverse problems: an example from carbon dioxide flux estimation, *Geosci. Model Dev. Discuss.*, 5, 3325-3342, doi:10.5194/gmdd-5-3325-2012, 2012.

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