Interactive comment on “Estimating surface CO$_2$ fluxes from space-borne CO$_2$ dry air mole fraction observations using an ensemble Kalman Filter” by L. Feng et al.

L. Feng et al.

Received and published: 27 February 2009

We thank all referees for their constructive comments on this paper. In our responses we address the main issues first and then the minor issues. Referee comments are shown in italics.

Replies to comments of Referee 1

Not required

Replies to comments of Referee 2

*In order to save computing time, the authors have reduced the dimension of the in-*
ference problem so much that one may wonder why the ensemble gain matrix (eq 6) is used in place of the true gain matrix (eq 3). The classical analytical computation would be more accurate and faster. An ensemble approach could be justified if the concentration error statistics were cycled from one window to the next, but this is no cycle here. Instead overlapping windows are used.

In this paper, we have described an ensemble Kalman filter for estimating surface fluxes from the upcoming OCO $X_{CO_2}$ observations. We have used a full-rank representation because theoretically it reliably estimates the a posteriori error covariance. Based on the calculations shown in the current paper, the spatial dimensions of our state vector are close to those that ensure that individual state vector elements are estimated independently. We acknowledge that this is probably due to the limitations of our simulation of $X_{CO_2}$ data using a relatively coarse resolution model. We anticipate that with real observations we should be able to independently estimate fluxes on smaller scales.

We have used overlapping windows with a length of $12 \times 8$ days, which cycle the error statistics, so that regional surface flux estimates can be constrained by a large amount of $X_{CO_2}$ observations made in a sufficiently long period (i.e., $12 \times 8$ days in the control run) afterwards. In general, the uncertainty associated with an estimated regional flux reduces rapidly with increasing number of assimilated observations, and becomes saturated after several 8-day assimilation cycles, which justifies our use of a short lag window (for example as short as 8 weeks).

Our results also showed that EnKF with a reduced-rank representation of the error covariance is able to accurately estimate regional fluxes. However, in agreement with other works (e.g., Peters et al., 2005), the reduced-rank representation tends to underestimate the uncertainties associated with the a posteriori, which would unnecessarily complicate our present discussion about error reduction from assimilating OCO observations.

In practice, this underestimation is also important to characterise when we start to use
real data, estimate surface fluxes on finer scales, and use a reduced-rank representation of the EnKF. There are approaches we can adopt to partially compensate such underestimations, and one example is included in the revised manuscript.

*It is said in lines 229 and 351 that the paper evaluated the EnKF approach, but this is hardly done. Given the same size of the problem, a proper evaluation would involve comparing the reduced-rank statistics with the full-rank matrix. Doing it is simple, as explained in point 1, and would greatly benefit the paper.*

In theory (Section 3.1-3.3), for our application, the deterministic ensemble transfer Kalman filter (ETKF) algorithm with a full-rank representation of the a priori error covariance is consistent with the ordinary Kalman filter both in the calculation of the gain matrix and in the calculation of the a posteriori error covariance for each individual assimilation cycle.

The use of a relatively short (12 weeks) lag window is justified by the insensitivity of the resulting a posteriori and the associated error covariance to using an even shorter lag window (8 weeks), as shown in our paper.

*The state vector is conveniently small in the presented EnKF, but no physical arguments are given in favour of this choice. It is just shown (section 4.5) that it has a strong impact. Can the prior error statistics be safely represented over the globe with just 144 regions?*

See above responses about the spatial dimension of the state vector. Regarding the error statistics, similar to other assimilation approaches (Chevallier et al., 2007a; Baker et al., 2006), we have had to make assumptions on the a priori error covariance. Our state vector includes 99 land regions with areas around several million km$^2$. Estimating these fluxes at a much finer spatial resolution using our simulated data is under-determined, showing large uncertainties and negative error correlations between neighbouring regions.
Minor points

L.25. The word “quantitative” has been removed.

L.28. We have replaced “in-situ” with “ground-based”.

L.89. The GEOS-Chem model resolution is chosen to be $2^\circ$ in latitude and $2.5^\circ$ in longitude.

L.99-100. We have changed the text to read: 'We use the full-physics retrievals assumed to be made at every 20 seconds...,'

L.129-135. We have added one sentence to point out that the measurement errors over land regions are usually much smaller than the uncertainties assigned to the model transport.

L.161. We changed the sentence as: OCO observations are only made in the daylight, and two consecutive orbits are separated by about $24^\circ$ in longitude. We assume that only observations made in one orbit are correlated with each other.

L.163. The uncertainties of the initial CO$_2$ states at the beginning of the experiment become progressively less important than the errors in the recent flux estimates as more data are ingested (Chevallier, et al., 2007a).

L.171. Changes have been made in Section 3.1 following the referees’ suggestions.

Eq.4. It represents a much simplified a priori error covariance.

L.184. In a full-rank representation, we can in principle calculate Jacobian $H$ using Eq.14. But such an explicit calculation of $H$ is unnecessary in our EnKF approach, and we only intend to use Eq.14 to avoid the re-run the GEOS-Chem model in our sensitivity experiments with different observation configurations. When a reduced-rank representation is used, calculation of $H$ via Eq.14 becomes invalid.

L.190. We have changed Section 3.1 following the suggestions.
L.211. We are using a deterministic approach (Zupanski et al., 2005) to construct the perturbation ensemble from singular value decomposition of the a priori error covariance.

L.264. Changed to: Despite their a priori errors being smaller than the typical values for the land surface fluxes.

L.282. “greater” is removed.

L.284. Changed “obscured” to “obscuring”.

L.298. Changed “geological” to “geographic”.

L.313. We agree that this result depends on the spatial resolution of the state vector, and include this point in the revised manuscript.

L.315. We have inserted the word “error” to avoid confusion.

L.326. “Weaker” means the comparison to the observations without correlations.

L.357. As mentioned before, our approach does not rely on the direct calculation of Jacobian.

Section 4.6: For a linear process like CO$_2$ transport in the atmosphere, the ensemble size only needs to be equal to (or smaller than) the size of the state vector to deterministically construct the perturbation flux ensemble as the representation of the error covariances.

L.376-383. We have now emphasised that our results are mostly consistent with previous studies, although our experiments are based on more realistic OCO observations. We also show that glint measurements provide important constraints to land-based surface CO$_2$ flux estimates, despite fewer clear observations and larger view spots compared to the nadir measurements.

L.389. We have added that sentence as suggested by the referee.
L.475/484. The typos are corrected.

L.489. Here, we are discussing about the reduced-rank representation with $N_x < N_e$.

Figure 6. Modifications have been made in both Figure 6 and its caption.

Replies to comments of referee 3

In this paper, we have described an ensemble Kalman filter for estimating surface fluxes from the upcoming OCO $X_{CO2}$ observations. In our control experiments, we have used a full-rank representation because it theoretically provides a reliable estimation of the a posteriori error covariance. At each individual assimilation cycle, our deterministic ensemble transfer Kalman filter (ETKF) algorithm with a full representation of the a priori error covariance is theoretically consistent with the ordinary Kalman filter in both the calculation of the gain matrix and the calculation of the a posteriori error covariance.

The use of a relatively short (12 weeks) lag window is justified by the insensitivity of the resulting a posteriori and the associated error covariance to using a shorter lag window (8 weeks), as shown in our paper.

In practice, our EnKF framework can be applied to estimate surface CO$_2$ fluxes at much higher spatial resolutions, such as the resolution of $4^\circ \times 5^\circ$ globally, when a reduced-rank representation of the error covariance is used to reduce computational costs. Our recent experiments (not shown) suggest that using as few as 170 ensemble members for each 8-day period, the EnKF approach can produce “realistic” land surface CO$_2$ flux estimates over grid boxes of $4^\circ \times 5^\circ$ from a perturbed a priori by assimilating OCO observations presented in the current paper. However, in agreement with other studies (e.g., Peters et al., 2005), a reduced-rank representation tends to underestimate the uncertainties associated with the a posteriori, which would complicate our discussions about error reduction from assimilating OCO observations.

We can, in principle, use certain approaches to compensate the underestimated un-
certainties and one example is included in the revision. But we agree with the referee that an accurate estimation of the a posteriori error covariance for inversions at much finer spatial resolutions is still a challenge to both the variational and the ensemble approaches.

Abstract, In 8. We have changed the sentence, as suggested.

P19920, In 90-13. We have changed the sentence.

P19922, eq(1). We have changed the formula.

P19924, In 7-8. In each individual assimilation step, we use the ensemble transform Kalman filter algorithm to calculate the ensemble gain matrix (Eq.6) and the transform matrix (Eq.10) from all clear observations made in the current 8-day period. We then update the surface flux estimates and the perturbation ensemble for a time period backwards to 12 weeks ago, using the resulting gain matrix and the transform matrix. We also update the ensemble of the 3-D CO$_2$ concentrations at the end of the current 8-day period, so that they are consistent with the new flux analysis (see Appendix B). We have added some sentences in section 3.1-3.2 to make these points clearer.

P19925, In 25. As mentioned before, we have used a full-rank representation to avoid the complications of the underestimated error covariance from using a reduced-rank approach in our discussions about error reduction.

But an explicit calculation of the Jacobian $H$ is not necessary in our ensemble approach.

P19926, In 10. We agree that it only provides an approximation if a reduced representation is used.

P19927, ln12-on. The posterior error covariance given by Eq.9 satisfies

$$P^a = (1 - KH)P^f.$$  \hspace{1cm} (1)
So, if a full-rank representation is used, this calculation is accurate, and consistent with the ordinary Kalman Filter.

P19928, In 25: It is not sensitive to the assumed true values of regional surface CO$_2$ fluxes, nor to the values of the perturbed CO$_2$ fluxes given as the a priori. We agree that it depends on the assumed a priori errors.

Figure 6. Here, we show the departures of the estimates from the “true” surface CO$_2$ fluxes, after being aggregated from 144 regions to the 22 TransCom-3 regions. For comparison, we also present the aggregated uncertainties of the a posteriori in the control run as the vertical lines (a factor of 1/2 have been missed in the original plot). Our EnKF use a lag window of 12×8 days, and the estimates for regional fluxes during Jan 17 and Feb 17 have been constrained by a large amount of observations made in a period from Jan.17 to roughly May 17. We have changed Figure 6 and its caption so that it is clearer for the readers.

P19930, In 22-23: See above replies on Figure 6.

Figure 9. It has been replotted to make the results for the control run clearer.

P19923, In 33: As discussed above, for each individual assimilation cycle, our approach is consistent with the ordinary Kalman filter when a full-rank representation of the error covariance is used. But the reduced-rank representation can underestimate the a posteriori errors.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 19917, 2008.