Interactive comment on “Estimating surface CO₂ fluxes from space-borne CO₂ dry air mole fraction observations using an ensemble Kalman Filter” by L. Feng et al.

D. Baker (Referee)
baker@cira.colostate.edu

Received and published: 22 January 2009

This study uses covariance estimates from an ensemble Kalman filter (EnKF) to estimate the constraint on surface CO₂ fluxes that are expected to be provided by measurements from NASA’s soon-to-be-launched Orbiting Carbon Observatory (OCO). For 8-day average fluxes at regional scales (99 land regions, 44 ocean regions, one low-flux ice-covered region), flux error reductions of generally over 50% are obtained over land, with weaker but still-significant reductions over the ocean obtained using glint-mode data. Glint data are found to provide an effective constraint for fluxes not only over the oceans (where the measurement precision is high) but also over the continents,
especially in the tropics, because of CO$_2$ flowing off the continents out over the ocean. These results are encouragingly similar to another recent OCO OSSE study (Baker, et al., ACPD 8, 20051-20112, 2008), that used a completely different inversion method, flux resolution, and measurement density. In both cases, the results should be viewed as providing potential "best-case" flux error reductions: a variety of systematic errors must be identified and removed from the OCO measurements before the relatively low random errors assumed will become dominant. A suite of sensitivity studies explore the dependence of the results on the proportion of glint- and nadir-mode data used, measurement biases, measurement density and correlations, the spatial resolution of the fluxes, and details of the ensemble filtering method.

Covariance estimates obtained from the spread of the filter ensemble are used in computing the error reductions. Mathematically, this is more satisfying than averaging estimate-truth flux differences over a small number of OSSE runs (as done in Baker, et al., 2008, and Chevallier, et al, JGR-Atmos., 112(D9), D09307, doi:10.1029/2006JD007375, 2007). However, it has been known for some time (and is nicely demonstrated here in one of the sensitivity studies) that the low-rank covariance estimates that ensemble filters give are generally poor at all but the coarsest space/time scales. To avoid this, the authors use a number of ensemble members equal to the dimension of the state (144 regions x 12 time steps in the state = 1768); in theory, this should give a full-rank covariance estimate. I imagine that the resolution of the fluxes estimated here has been chosen to be somewhat coarse on purpose so that the number of ensemble members is manageable. That is fine for the purposes of doing this OSSE study, but it is of course not how the ensemble filters will be used in actual practice. One of the main points of using an ensemble Kalman filter, instead of some flavor of the traditional, full-rank Kalman filter, is that large problems then become computationally tractable. In such cases, the number of ensemble members is generally much smaller than the dimension of the state, in order to achieve the computational savings. Thus, it is somewhat overstating the case to say (as is done here in the conclusions) that one of the main advantages of the EnKF is that it "provides a framework to esti-
mate the uncertainty of a posteriori fluxes": when used as it usually is, with relatively few ensemble members, it provides only a low rank covariance estimate, which the authors show in Figure 9 gives a poor, over-optimistic view of the errors. The variational methods can provide a similarly poor, low-rank covariance estimate, as well.

The authors do a nice job of exploring how the results depend on the ensemble size and the flux time window. One thing that is not explored, and which might be a nice addition in the final paper, is how accurate the full-rank covariance results are compared to what would be given by a traditional, full-rank Kalman filter. With a matrix size of 1768x1768 here, and with about 27 time steps across 7 months, the computational cost of running a traditional Kalman filter would not be overly burdensome. The approximations involved in deriving the ensemble filter may well introduce errors that would cause even the full-rank covariance from the ensemble to be off by quite a bit.

In general, this is a well-written and interesting paper, and ought to be published in ACP. I have a few detailed questions below that could be clarified in the final version.

Detailed comments:

Abstract, line 8: it is not just the prior but also the posterior error covariances that are approximated by the ensemble. Maybe reword as "to represent the error covariance of the 8-day CO2 surface fluxes over 144..."

p 19920, ln 9-13: These two studies are really distinguished by: 1) constant measurement errors (1 or 2 ppm) everywhere, with the Chevallier references removing data when clouds are present), and 2) flat weighting in the vertical. The distinction between nadir and glint would have come in mainly in the location of the ground tracks, and I am not sure how closely this was controlled in those papers.

p 19922, eq (1): the use of the term (1/(1-w)) in this matrix equation is not good form. Replace it with some equivalent matrix form.

p 19924, ln 7-8: The observations are binned in 8-day blocks for the purposes of the
filter. It is not clear whether the observations are modeled at the time they occur within the 8-day span, however – are they? (Figure 4 suggests they are.) Does the covariance represented by $P^f$ in equation (3), used to calculate $K$, stay constant across the 8-day span, or does it vary across the span, to permit better accuracy when computing $HP^f$ for each measurement? Some description of how the covariance is propagated in time might be in order here (is any dynamical error added from time step to time step, to increase the spread in the ensemble?).

p 19925, In 25: to avoid explicitly having to calculate $\partial H/\partial x$ is one reason to replace the covariance matrix with the ensemble; the other big reason is to avoid having to form a full-rank covariance matrix in the first place.

p 19926, In 10: again, for all cases in which the number of ensemble members is less than the state dimension, equation (9) gives only a low-rank approximation of the full covariance.

p 19927, In 12-on: Another good reason for comparing the approximate covariance to the exact covariance from the full-rank, traditional Kalman filter is that errors introduced by approximations such as this one may be quantified.

p 19928, In 25: As can clearly be seen in equation (15), the error reduction does indeed depend on assumptions made about the prior fluxes: it depends on the a priori flux uncertainty $\sigma^f$. If the prior uncertainties are made large enough, the error reduction approaches 100%, regardless of the information provided by the measurements. This is a problem with the error reduction statistic, but nevertheless it has proved useful enough that most people tend to use it.

Figure 6 caption, In 4: "Vertical lines denote the standard deviation of the error." If this is the a posteriori error, maybe you could add "a posteriori" here so that this is very clear. I am somewhat surprised that these a posteriori uncertainties increase and decrease as they do. I would expect a gradual decreasing of the uncertainty as time goes on, as the a priori uncertainty dies away under the influence of an increasing number of
measurements. Does this a priori uncertainty die off so quickly (before 17 days, ie. Jan 17th)? What level of dynamical error are you adding?

p 19930, In 22-23. Why are the actual errors in Figure 6 so much smaller than the a posteriori uncertainty estimates? One would expect these to be roughly comparable.

Figure 9b: Please redraw this figure so that we can see where the control experiment results (the black circles) fall.

p 19933, In 33: The EnKF "... provides a framework to estimate the uncertainty of a posteriori fluxes." Again, this is only the case when enough ensemble members are used to provide a full-rank covariance estimate (ie. when a number equal or greater than the state dimension are used). And we cannot even be sure of this, since the ensemble covariance estimate has not been compared to the full-rank covariance from the traditional Kalman filter here. In the general case, all one can say is that the covariance estimates might be useful at the coarsest scales.

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