## Anonymous Referee #1

Interactive comment on "A Global Carbon Assimilation System using a modified EnKF assimilation method" by S. Zhang et al.

#### **Acknowledgements**

The authors gratefully acknowledge the anonymous referee #1 for his constructive and relevant comments, which lead to much improvement of this manuscript. We have checked our work carefully according to these comments and made the suggested changes.

#### **General Comments**

The authors present their data assimilation system GCAS-EK, which is based on the application of a Kalman Filter to the CO2 flux estimation problem. Some recent improvements to such systems were incorporated into this version, such as the inflation of covariances (on fluxes and observations) and the replacement of the forecast statistics with a better one, based on the analysis state vector mean. This system is described in a rather short description, that mostly states that all input data and settings were copied from NOAA/ESRL's carbon tracker website. One important difference with carbon tracker itself is the choice to also place CO<sub>2</sub> in the state vector, which has been demonstrated to be beneficial in a joint meteorological-CO2 data assimilation method, which GCAS-EK is however not. The impact of the innovations in the extended state vector, inflation estimation, and forecast statistics are demonstrated in straightforward experiments, much similar to the original publication of these methods. Following these OSSE's, a real global CO2 inversion is performed with as main result a better fit to the observed CO2 that was assimilated, and closer agreement to the published carbon tracker results at global, and at TransCom scales. Overall, I feel that this new system has a place in the ranks of current CO2 data assimilation methods, but the current paper does not highlight much novelty, does not convincingly show the added value of an extended state vector or shorter assimilation window, and does not demonstrate that this system is mature enough to estimate global carbon fluxes to a level of reliability comparable to existing methods. This is a consequence of the way the paper is structured: it does not fully document your system as I would expect for GMD, it also does not fully assess the details of extended state vectors or window lengths as could be suitable, and it also is not a sufficient paper to show you can estimate good carbon fluxes. The latter would be an interesting paper even for ACP or BG I believe. A clearer choice of the aim of this paper would in that sense help a lot.

#### **Our reply:**

Thank you for your valuable comments. Please see our reply to your following specific comments.

The paper is very well written in appropriate English, and structured logically which makes it easy to read. Sufficient literature from the field is cited, although there are some blatant omissions in referencing data

source as documented under (1). I think the design and application of this system is of interest to the GMD reader community, if the following four major points of concern are addressed in a next manuscript:

This paper cannot be published without consent and acknowledgement of the CO2 data providers. You currently state that you got the data from the carbon tracker website but this is not an acceptable citation, nor the right source to get observational data. The data used by carbon tracker is owned by many individual PIs and the terms of use of this data state that these must all be informed when you use their data, and consulted to discuss acknowledgement. This has clearly not been done yet, and this must be rectified. Along a similar line, this study uses many products and details obtained from the carbon tracker website, but there is no acknowledgement for the carbon tracker effort as asked for on their website. Nor is there any reference to the original fossil, fire, and ocean flux data providers behind carbon tracker that also should receive fair credit for their work. I find this scientifically unacceptable.

## **Our reply:**

Thank you for your comments.

We have added all the sources of the datasets we can find on the website in the following paragraphs and will send the manuscript to data owners to ask how to acknowledge them as soon as the manuscript is

completed. We promise that all the mistakes you mentioned will be rectified. In the revised manuscript,

"The vegetation fire flux is taken from CarbonTracker 2011 dataset, which is modeled using the Carnegie-Ames Stanford Approach (CASA) biosphere model (Potter et al., 1993) based on the Global Fire Emission Database (GFED) (van der Werf et al., 2006)."

"The oceanic  $CO_2$  flux is taken from CarbonTracker 2011 optimized results, whose a priori estimates are based on two different datasets: namely ocean inversions flux result (Jacobson et al., 2007) and p $CO_2$ -Clim prior derived from the climatology of seawater p $CO_2$  (Takahashi et al., 2009)."

"The fossil fuel combustion estimate is the dataset preprocessed by CarbonTracker 2011 from the global total fossil fuel emission of the Carbon Dioxide Information and Analysis Center (CDIAC) (Boden et al., 2011) and the "ODIAC" emission dataset (Oda and Maksyutov, 2011)."

"The atmospheric  $CO_2$  concentration measurements collected and preprocessed by Observation Package (ObsPack) Data Product (Masarie et al., 2014) are used in this study (Product Version: obspack\_co2\_1\_CARBONTRACKER\_CT2013\_2014-05-08). The selected  $CO_2$  measurements on 92 sites include observations of two main types: the measurements of air samples at surface sites and in situ quasi-continuous  $CO_2$  time series from towers. Since some stations have

multiple observations within a week, on average there are about 140 observations every week during 2002 and 2008. Six laboratories (NOAA Global Monitoring Division, Commonwealth Scientific and Industrial Research Organization, National Center For Atmospheric Research, Environment Canada, Lawrence Berkeley National Laboratory and Instituto de Pesquisas Energeticas e Nucleares) provided these measurements and information of observation sites used in this study is listed in Table 1."

And in the Acknowledgement:

"We acknowledge all atmospheric data providers to obspack\_co2\_1\_CARBONTRACKER\_CT2013\_2014-05-08, and those contribute their data to WDCGG. We grateful acknowledge CarbonTracker CT2011 results provided by NOAA ESRL, Boulder, Colorado, USA from the website at http://carbontracker.noaa.gov."

(2) Technically, the tests shown are not so interesting because they demonstrate improvements that were already described in more detail in previous publications. Their application in GCAS-EK is not much different from those papers and yields results which are quite predictable. Moreover, some of the questions that are important to the real-world application of GCAS-EK are not answered in this test. These questions are: (1) Why would the extended state vector be expected to outperform the

regular flux state vector if they are fully related through a linear operator G? and (2) How much carbon mass is lost or gained per cycle/season/year due to the adjustments made directly to the mixing ratios rather than to the underlying fluxes? I recommend that the authors try to answer these questions as a prelude to the real-world application of estimating CO2 with GCAS-EK.

## **Our reply:**

Thank you for your comments.

Following your advice, we have deleted Section 4 of "simulation study".

We would like to answer Question (2) first. In this study, the background  $\mathrm{CO}_2$  concentration field at the beginning of a week is the analysis state at the end of the previous week. It is then updated using the observations within the week, so the estimated  $\mathrm{CO}_2$  concentration at the beginning of the week is different from that at the end of the previous week. This results in inexact carbon mass balance. To remove the imbalance, a corrected atmospheric  $\mathrm{CO}_2$  concentration can be generated using the sequential forecast of  $\mathrm{CO}_2$  concentration with the optimized carbon fluxes starting from the very beginning of the whole assimilation period. The corrected  $\mathrm{CO}_2$  concentration is denoted by  $\mathbf{c}_i^{\mathrm{ca}}$ . By this way the carbon mass can be balanced.

For question (1): Given an atmospheric transport model and its

meteorological forcing data, the CO<sub>2</sub> concentration field is fully determined by the "initial condition" and "boundary conditions". In fact, if we have to find a state vector of "minimum length", it will consist of the initial CO<sub>2</sub> concentration field and the scaling factors. If the initial condition is inaccurate, there will be error in forecasted observations. There are two ways to reduce this error: one is using an assimilation window long enough to decrease the impact of the error of the initial CO<sub>2</sub> concentration field, which is done by CarbonTracker and many atmospheric inversions etc.; another is to optimize the initial CO<sub>2</sub> concentration field with observations, which is carried out by *Kang et al.* (2011,2012), *Liu et al.* (2012), *Miyazaki et al.* (2011) and this study. If a short assimilation window is used (for example, one week in this study), the error of the initial condition cannot be ignored. This is the main reason we include the CO<sub>2</sub> concentration field in the state vectors.

The benefit of this inclusion needs to be tested against the traditional approach without this inclusion. This issue is studied with the one-week assimilation window. A comparative experiment is designed as follows. At every time step, the  $CO_2$  concentration is not updated. For maintaining the  $CO_2$  mass balance, the analysis  $CO_2$  concentration is derived by sequentially predicting atmospheric  $CO_2$  concentration forced by the updated flux within the week. The results showed that the overall RMSE of analysis  $CO_2$  concentration observations in this experiment is

8.5% larger than that of the corrected analysis  $CO_2$  concentration  $\mathbf{c}_{t}^{ca}$  by GCAS-EK. This suggests that inclusion of  $CO_2$  concentration in state vectors can significantly alter the  $CO_2$  mass balance and may have advantage in optimizing the surface  $CO_2$  flux.

If the  $CO_2$  concentration is not included in state vectors, the analysis  $CO_2$  concentration at the beginning of each week is just the analysis  $CO_2$  concentration at the end of the previous week, so the  $CO_2$  concentration observations within the current week are not used to optimize the  $CO_2$  concentration at the beginning of each week. However, when the  $CO_2$  concentration is included in state vectors, all the observations within the current week and the previous weeks are used to estimate the  $CO_2$  concentration at the beginning of the current week. So the  $CO_2$  concentration at the beginning of each week estimated by inclusion of  $CO_2$  concentration in state vectors could be more accurate than that estimated in the no inclusion case. Therefore, the estimated flux associated with the updated  $CO_2$  concentration at the beginning of current week could have better quality. This is demonstrated by smaller RMSE with the inclusion than that without the inclusion.

Most of discussions above have been added in the revised manuscript. Please see the manuscript file for the revision.

#### References

Kang, J. S., Kalnay, E., Liu, J., Fung, I., Miyoshi, T., and Ide, K.: "Variable localization" in an ensemble Kalman filter: Application to the carbon cycle data assimilation, J. Geophys. Res., 116, D09110, 2011.

Kang, J. S., Kalnay, E., Miyoshi, T., Liu, J., and Fung, I.: Estimation of surface carbon fluxes with an advanced data assimilation methodology, Journal of Geophysical Research: Atmospheres (1984–2012), 117, 2012.

Liu, J., Fung, I., Kalnay, E., Kang, J.-S., Olsen, E. T., and Chen, L.: Simultaneous assimilation of AIRS Xco2 and meteorological observations in a carbon climate model with an ensemble Kalman filter, Journal of Geophysical Research: Atmospheres, 117, D05309, 10.1029/2011JD016642, 2012.

Miyazaki, K., Maki, T., Patra, P., and Nakazawa, T.: Assessing the impact of satellite, aircraft, and surface observations on CO2 flux estimation using an ensemble-based 4-D data assimilation system, J. Geophys. Res. [Atmos.], 116, D16306, 10.1029/2010JD015366, 2011.

(3) You have chosen to apply your method globally, yet you use your Kalman Filter as a filter rather than a smoother. The only justification you give is that transport is uncertain and various choices are possible. This is not enough in my opinion. If you want to apply your system globally, you need to show that a filter captures the signals of CO2 sufficiently well in that period, and that going to a longer window or a lagged window has little advantage. My estimate is that your one week filter is too short for global flux estimates, and is partly responsible for the large flux differences with carbon tracker in your figures.

## **Our reply:**

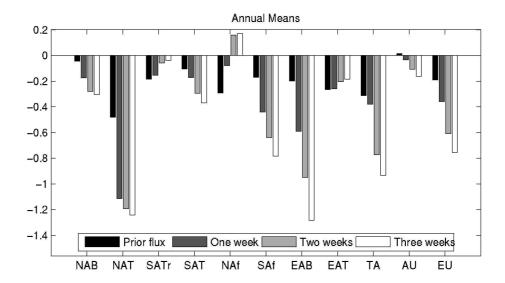
Thank you for your comments.

Different lengths of the assimilation time window are used in various systems (5 weeks in CarbonTracker, 3 and 7 days in *Miyazaki et al.* (2011) and 6 hours in *Kang et al.* (2012)). We choose the one-week assimilation

window in our methodology for the following three reasons. First, since most surface stations only have weekly observations, we need at least one week data to cover the globe. Second, beyond one week the errors of the atmospheric transport model may be significant, but they are very difficult to quantify. Third, the detailed information of observations may be attenuated with time by atmospheric diffusion and advection (*Enting*, 2002).

For comparison to longer assimilation windows, the following alternative experiments with moving assimilation windows were carried out. In the first alternative experiment, the length of the moving window is set to be two weeks while the forecast time step is still one week. The CO<sub>2</sub> concentration observation system is still the same as that described in Section 3, but is used to update the global carbon flux and the atmospheric CO<sub>2</sub> concentration within the current week and the previous week. This procedure is similar to GCAS-EK, which provides the ensemble forecast state of the first week in the assimilation window that is set as its ensemble analysis state at previous assimilation time step. Therefore carbon fluxes and CO<sub>2</sub> concentration every week is optimized twice with the observations in the current week and the next week. The corrected analysis of CO<sub>2</sub> concentration is also retrieved from rerunning the atmospheric transport model. The second alternative experiment is similar to the first one, but with the three-week moving window.

The linear trends of the observations, the corrected CO<sub>2</sub> concentrations averaged over all observation sites with one-week, two-week and three-week moving windows are 2.14ppm yr<sup>-1</sup>, 2.17 ppm yr<sup>-1</sup>, 1.59 ppm yr<sup>-1</sup>, 1.13 ppm yr<sup>-1</sup>, respectively. It seems that the longer the moving window is, the larger difference is the long term growth to the measurements. For further investigating the reason, the annual mean carbon budgets on 11 Transcom regions are shown in Fig. R1. It can be found that the longer the moving window is, the larger are the carbon budget adjustments. Long windows result in underestimation of the corresponding long term growth rate. These facts indicate that the one-week assimilation window may be most appropriate. Incidentally, the corresponding trend for CarbonTracker 2011 is 2.15 ppm yr<sup>-1</sup>, also very close to the trend observed.



**Figure R1**. Annual means of carbon budgets (PgC yr<sup>-1</sup>) on 11 Transcom regions in four different cases. Four cases are associated with prior values modeled with ecosystem model BEPS, assimilated results using GCAS-EK with one-week assimilation windows, two-week windows and three-week windows. 11 regions in

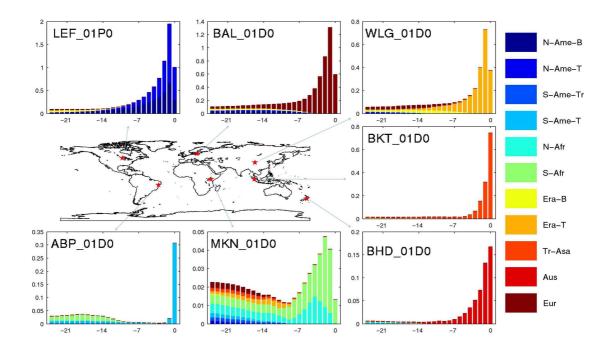
X-axis refer to 'North American Boreal' (NAB), 'North American Temperate' (NAT), 'South American Tropical' (SATr), 'South American Temperate' (SAT), 'Northern Africa' (NAf), 'Southern Africa' (SAf), 'Eurasia Boreal' (EAB), 'Eurasia Temperate' (EAT), 'Tropical Asia' (TA), 'Australia' (AU) and 'Europe' (EU), respectively.

To further investigate the long time and long distance impact of atmospheric transport on  $CO_2$  observations, components of  $CO_2$  concentration at observation sites associated with different Transcom regions in each day before their observation times are calculated in the following way. For a given region and some day before the observation time, prior fluxes on other regions and in other days are all masked. Then the atmospheric transport model can be run with a homogeneous initial atmospheric  $CO_2$  concentration and forced by the masked fluxes to obtain the corresponding  $CO_2$  concentration components.

These components at individual sites are then averaged in time to investigate general impacts of carbon fluxes from different sources. Results at 7 selected sites are shown in Fig. R2. For these sites, CO<sub>2</sub> concentrations resulting from carbon fluxes within 25 days are mainly from local carbon fluxes within 7 days (although mostly within 3 days). Carbon fluxes beyond 7 days or regions far from observation locations have very small impacts, indicating that they have little information in observations (i.e. the contribution is less than observation error), even if the atmospheric transport model is accurate. Actually the majority of continental observation sites used in this study (approximately 49) have

similar properties to these 7 sites. If the errors of the transport and ecosystem models are considered, the information of fluxes one week before may be even more difficult to estimate.

The setting of length of the assimilation window is closely related to spatial and temporal localizations of forecast errors. For the observation network and the atmospheric transport model used in this study, the one-week assimilation window seems most suitable.



**Figure R2.** Mean components of CO<sub>2</sub> concentration at observation sites (Site IDs: LEF\_01P0, BAL\_01D0, WLG\_01D0, BKT\_01D0, BHD\_01D0, MKN\_01D0 and ABP\_01D0) from 11 Transcom regions in each of 25 days before the observation time. X-axis refers to days before the observation time. Y-axis refers to the amount of CO<sub>2</sub> concentration in ppm. Different colors within a bar refer to CO<sub>2</sub> concentration from 11 different Transcom regions. 11 regions refer to 'North American Boreal' (N-Ame-B), 'North American Temperate' (N-Ame-T), 'South American Tropical' (S-Ame-Tr), 'South American Temperate' (S-Ame-T), 'Northern Africa' (N-Afr), 'Southern Africa' (S-Afr), 'Eurasia Boreal' (Era-B), 'Eurasia Temperate' (Era-T), 'Tropical Asia' (Tr-Asa), 'Australia' (Aus) and 'Europe' (Eur), respectively.

#### References

Enting, I. G.: Inverse Problems in Atmospheric Constituent Transport, Cambridge University Press, New York, 2002.

Kang, J. S., Kalnay, E., Miyoshi, T., Liu, J., and Fung, I.: Estimation of surface carbon fluxes with an advanced data assimilation methodology, Journal of Geophysical Research: Atmospheres (1984–2012), 117, 2012.

Miyazaki, K., Maki, T., Patra, P., and Nakazawa, T.: Assessing the impact of satellite, aircraft, and surface observations on CO2 flux estimation using an ensemble-based 4-D data assimilation system, J. Geophys. Res. [Atmos.], 116, D16306, 10.1029/2010JD015366, 2011.

(4) The real-world application of the system is interesting, but I feel that the assessment of its realism needs to be expanded significantly. Now, we are just given a comparison to carbotracker fluxes that shows large differences but little evaluation. In the end, the question whether your system can produce good fluxes that match atmospheric concentrations well is not answered for me. The authors should look more closely at the evaluation of other systems that have recently been published such as from Liu et al., (2013) and Zhang et al., (2013). Important is to include an evaluation of mixing ratios, both those assimilated and non-assimilated such as from aircraft or other sites. And to assess these at multiple time scales (diurnal, syncopic, seasonal, annual) and multiple location (tropics, SH, NH). Then, the sum of fluxes must be given for the globe and their sum must be compared to the global CO2 growth rate. Next, these must be split into ocean and land fluxes, and the land fluxes must be looked at to see where the land sink

appears largest (tropics, NH boreal, or NH temperate, and Europe vs Asia vs North America). These must then also be split into forests and grasslands or cropland uptake. If all of these look good, a comparison can be made to the results of other systems, such as those in TransCom, or RECCAP, and perhaps carbon tracker. And again, this has to be done on seasonal, annual, and interannual scales. Finally, independent assessment against for instance GCP estimates, or eddy-covariance, or crop yields, or forest surveys could help. I realize this is not an easy task, but to publish a new inversion system one has to convince the existing community of its realism.

# **Our reply:**

Thank you for your comments.

The purpose of this study is to show some ideas that are potentially useful in assimilating atmospheric CO<sub>2</sub> concentration measurements into ecosystem models, including the inclusion of atmospheric CO<sub>2</sub> concentration in state vectors, the implementation of the Ensemble Kalman Filter (EnKF) with a short assimilation window, the use of analysis states to iteratively estimate ensemble forecast errors, and a maximum likelihood estimation of the inflation factors of the forecast and observation errors. We plan to put the assessment of the system into another manuscript, which is similar to the papers you mentioned (Liu et al., 2014; Liu et al., 2012; Zhang et al., 2014).

Following your advice, we have added more assessment in the revised manuscript. First, Chi-square tests were carried out to directly investigate the effectiveness of the techniques used to improve the estimation of forecast and observation error covariances. Second, long-term growth rates in several cases were tested and compared. Third, independent gridded net ecosystem productivity data such as that by Xiao et al. (2011) was compared to that by GCAS-EK. Xiao's data is based on eddy covariance and MODIS data.

Unfortunately, we carried out the assimilation from 2002 to 2008, when there is little aircraft or satellite data. Furthermore, direct carbon flux observations such as eddy covariance are sparse over the globe and their spatial representativeness is very limited, and thus they are not suitable for comparisons with our gridded results, although tower flux data at more than 100 stations are used to optimize the BEPS model that is used to produce the prior land surface carbon flux.

In the future, we are going to extend our assimilation to recent years using more observations, and comprehensive and systematic assessments of the methodologies developed in GCAS-EK will carried out.

#### References

Liu, J., Fung, I., Kalnay, E., Kang, J.-S., Olsen, E. T., and Chen, L.: Simultaneous assimilation of AIRS Xco2 and meteorological observations in a carbon climate model with an ensemble Kalman filter, Journal of

Geophysical Research: Atmospheres, 117, D05309, 10.1029/2011JD016642, 2012.

Liu, J., Bowman, K. W., Lee, M., Henze, D. K., Bousserez, N., Brix, H., Collatz, G. J., Menemenlis, D., Ott, L., Pawson, S., Jones, D., and Nassar, R.: Carbon monitoring system flux estimation and attribution: impact of ACOS-GOSAT X CO 2 sampling on the inference of terrestrial biospheric sources and sinks, 2014, 10.3402/tellusb.v66.22486, 2014.

Zhang, H. F., Chen, B. Z., Machida, T., Matsueda, H., Sawa, Y., Fukuyama, Y., Langenfelds, R., van der Schoot, M., Xu, G., Yan, J. W., Cheng, M. L., Zhou, L. X., Tans, P. P., and Peters, W.: Estimating Asian terrestrial carbon fluxes from CONTRAIL aircraft and surface CO2 observations for the period 2006–2010, Atmos. Chem. Phys., 14, 5807-5824, 10.5194/acp-14-5807-2014, 2014.

Xiao, J., Zhuang, Q., Law, B. E., Baldocchi, D. D., Chen, J., Richardson, A. D., Melillo, J. M., Davis, K. J., Hollinger, D. Y., Wharton, S., Oren, R., Noormets, A., Fischer, M. L., Verma, S. B., Cook, D. R., Sun, G., McNulty, S., Wofsy, S. C., Bolstad, P. V., Burns, S. P., Curtis, P. S., Drake, B. G., Falk, M., Foster, D. R., Gu, L., Hadley, J. L., Katul, G. G., Litvak, M., Ma, S., Martin, T. A., Matamala, R., Meyers, T. P., Monson, R. K., Munger, J. W., Oechel, W. C., Paw, U. K. T., Schmid, H. P., Scott, R. L., Starr, G., Suyker, A. E., and Torn, M. S.: Assessing net ecosystem carbon exchange of U.S. terrestrial ecosystems by integrating eddy covariance flux measurements and satellite observations, Agricultural and Forest Meteorology, 151, 60-69, <a href="http://dx.doi.org/10.1016/j.agrformet.2010.09.002">http://dx.doi.org/10.1016/j.agrformet.2010.09.002</a>, 2011.

My recommendation is that the current MS is rejected and that the authors work on this manuscript some more before resubmitting it, since the changes I ask for are beyond a simple major revision. The first part of the paper should then focus on demonstrating that the extended statevector is an asset to this system and not just a liability for loss of CO2 mass. Also, it should demonstrate that the non-smoother version of the EnKF that they apply here is suitable for doing global inversions. Then, the global inversion should be presented, benchmarked in the method as described above under point (4). I hope my further comments on the manuscript in PDF help this effort.

## *In the supplement:*

(1) Title: This title is a bit awkward as it contains the word assimilation twice, also the acronym EnKF is not known to all readers.

Carbon Assimilation for many persons refers to the process of carbon fixation by photosynthesis. I suggest the authors make a better title.

## **Our reply:**

Thank you for your comments. We have changed the title to "A Global Carbon Assimilation System using a modified Ensemble Kalman filter".

(2) P6520, L25: I am not sure I agree with this reasoning that including the  $CO_2$  concentrations in the state vector should improve carbon flux estimations. How would that help? In principle, the  $CO_2$  concentrations are fully determined by the surface fluxes, so putting them both in the state vector is not so intuitive to me. Of course, the reason they did go this direction is because the relationship between surface fluxes and atmospheric  $CO_2$  is given by a transport model with uncertainties and putting  $CO_2$  in the state vector allows you to correct for biases in transport, and also reduces the need to explicitly simulate the  $CO_2$ -flux relationship over long time periods.

## Our reply:

Thank you for your comments. Please see our reply to the Question

## (1) of your Major Comment 2.

(3) P6521, L25: In Kang et al (2011, 2012) and Liu et al (2012,2013)  $CO_2$  concentrations are added to the state vector because they have strong correlations with weather variables that are simultaneously assimilated. This is much different from this study and the one by Miyazaki where only fluxes and  $CO_2$  are added. This difference should be noted explicitly in the text.

## **Our reply:**

Thank you for your comments.

We have added the following sentence in the Introduction section of revised manuscript,

"Kang et al. (2011) and Liu et al. (2012) also added  $CO_2$  concentration to the state vectors due to their strong correlations with weather variables that are simultaneously assimilated."

(4) P6522, L10-15: Can you add a reference (URL or paper) to this source, as well as some form of acknowledgement for using this product? And note that NOAA/ESRL is often not the owner of these datasets themselves and true references should be made to the original data providers such as CDIAC, GFED, etc...

## **Our reply:**

Thank you for your comments. Please see our reply to your Major Comment 1.

(5) P6522, L14: "rests" to "rest"

Our reply: Correted.

(6) P6522, L20: Please also mention the lack of knowledge on historical land-use change and land management, as this likely exceeds parameter uncertainties.

## **Our reply:**

Thank you for your comments.

We have rewritten this sentence in the revised manuscript,

"Errors in these parameters lead to biases of model results (Other uncertainties, such as lack of knowledge on historical land-use change and land management, also have influence on model results)."

(7) P6523, L20: This is not acceptable as reference for the measurements used in this study. Carbontracker is not the source of this data and its is stated very explicitly that the original data owners must be contacted when these datasets are used in a publication. Then they must be asked how to be acknowledged. Simply downloading the data from a

website is not the way to go in our field. Please rectify this mistake.

## **Our reply:**

Thank you for your comments. Please see our replay to your Major Comment 1.

(8) P6523, L25: What do you mean with "chosen to fit the observations?" Variances are not the same as mixing ratios...

## Our reply:

Thank you for your comments.

We mean the "model-data mismatch" error in *Peters et al.* 2005. In the revised manuscript, the sentence is rephrased as:

"They were subjectively chosen and manually tuned to fit into specific atmospheric transport models and observations."

#### Reference

Peters, W., Miller, J. B., Whitaker, J., Denning, A. S., Hirsch, A., Krol, M. C., Zupanski, D., Bruhwiler, L., and Tans, P. P.: An ensemble data assimilation system to estimate CO2 surface fluxes from atmospheric trace gas observations, J. Geophys. Res. [Atmos.], 110, D24304-D24304, 10.1029/2005JD006157, 2005.

(9) P6524, L13: But in this setup, the spread in Ci simply reflects the spread in fluxes and the concentration variance is fully correlated with the flux errors. This is different from the methods in Kang et al (2012) and Liu et al (2012,2013) where  $CO_2$  concentrations are added to the

state vector because they have strong correlations with weather variables. This difference should be noted explicitly in the text. The question becomes: why do you expect this method to work better than just having fluxes in the state vector? After all, the observations you have are not different, and the relation between fluxes and concentrations is fully explicit through G

## **Our reply:**

Thank you for your comments.

Ci (4-Dimensional: 3D in space and 1D in time) reflects the spread both in fluxes (3D: 2D in space and 1D in time) and the initial  $CO_2$  concentration field (3D in space) at the beginning of the week. The concentration covariance is also correlated to both the error of the initial  $CO_2$  concentration field and flux errors. Since we are using a relatively short assimilation window, the error in the initial  $CO_2$  concentration field is significant to the concentration covariance and we are trying to reduce this error by including  $CO_2$  concentration in the state vectors.

Please see our reply to your Major Comment 2 for more details.

#### (10) P6528, L9

### **Our reply:**

Thank you for your comments. We have deleted the whole section following your comment.

## (11) P6530, L7

## **Our reply:**

Thank you for your comments. We have deleted the whole section following your comment.

P6530, L19: I am not surprised that the extended state vector (12)does not really help as it contains no new information than the CO<sub>2</sub> observations you already had before, and it is fully correlated to the fluxes. The gain of time for not having to rerun the model forward must be weighed against the 'inexact mass balance': by adding or subtracting CO<sub>2</sub> from the atmosphere without a corresponding surface flux adjustment, you are creating CO₂ that is not accounted for by exchange between reservoirs. On longer time scales, this balance is very important. I suggest that you calculate this balance for your system by: (1) calculating per time step the change in mass of atmospheric CO<sub>2</sub> (2) calculating as well as the surface flux for that step (3) and compare these to each other to estimate the amount of 'ghost-CO<sub>2</sub>' created in each step. If this number is small (say <1%) of surface flux then this issue might be minor. (4) Then, also compare this on an annual basis: does the ghost-CO2 add up over time to a substantial flux, or does it average out over a year? And does it have a seasonal pattern?

# **Our reply:**

Thank you for your comments. Please see our reply to Question (2) of your Major Comment 2.

(13) P6531, L4: The details should go to the method section.

## Our reply:

Thank you for your comments. We have moved them to the methodology section.

(14) P6532, L10: You are describing here in words things that the reader can see in the figure. But what I expect is not a description, but an explanation of the differences: why are these fluxes not the same as carbontracker when you have copied almost the whole setup (observations, prior fluxes, variances, initial conditions, scaling factors)?

# **Our reply:**

Thank you for your comments.

Although we have used the same observations and variances and initial conditions since the very beginning at 1<sup>st</sup> Jan, 2002 as well as a similar setting of scaling factors, the system is still very different from CarbonTracker in many aspects, such as prior ecosystem carbon fluxes (modeled with BEPS in this study vs CASA in CarbonTracker), data assimilation methodology (with several new developments of Ensemble

Kalman filter), length of the assimilation window (one week in this study vs 5 weeks in CarbonTracker) etc. Since the observation network is not dense enough to constrain the carbon fluxes that are inverted, small changes in system settings may lead to large differences in the results. Without a large set of modeling experiments and verification of independent estimates, it is difficult to give an exact explanation of the improvements in the optimized flux due to the introduction of new methodologies in GCAS-EK. We will put more effort on this issue and hope we can tell more on the reasons in the future.

We have deleted the unnecessary descriptions to the figure to make the manuscript more concise.

## (15) P6545: Where are the error bars on these fluxes?

### Our reply:

Thank you for your comment. We have added the error bars on the figure. With the ensemble methodology, we can get an ensemble of these fluxes and the corresponding errors are calculated as the spread of this ensemble.

## P. Rayner (Referee) prayner@unimelb.edu.au

Interactive comment on "A Global Carbon Assimilation System using a modified EnKF assimilation method" by S. Zhang et al.

#### **Acknowledgements**

The authors gratefully acknowledge Prof P. Rayner for his constructive and relevant comments, which helped greatly in improving the quality of this manuscript. We have checked our work carefully according to these comments and made the suggested changes.

#### **General Comments**

This paper presents a new inversion method for CO2 fluxes and applies it to the period 2002–2008. The novelty in the method is the inclusion of CO2 concentration in the state vector allowing the relaxation of the perfect model assumption for transport. The ensemble method used makes this large augmentation of the state vector possible. The explicit treatment of transport error as part of the forecast error also allows better treatment of the observational error since this is now much closer to the observations (previously it was dominated by errors in the transport model). The paper also introduces to Ensemble Kalman Filter inversions the techniques of objective estimation of covariance scaling parameters. These are called inflation parameters in this study but play the same role as the scaling parameters of Michalak et al. (2005). Incidentally I think this paper should be cited. No doubt the authors came to their objective function via the KF literature but a citation would point out the familiarity of the approach to the conventional atmospheric inverse community.

The paper makes an important methodological contribution. It is well written and, most pleasingly, the algorithm is clearly enough described that it could be copied by someone with reasonable knowledge of the field. Analysis of the results is less developed but this is GMD and hopefully this can be taken up at a later date. I have no overall suggestions for the paper but do suggest a couple of small extra pieces of analysis in the specific comments below.

## **Our reply:**

Thank you for your valuable comments.

The inflation parameters in this study do play the same role as the scaling parameters in *Michalak et al. (2005)*.

We have cited *Michalak's paper* in the revised version and added the following sentence in 2) Error Step of Section 3.1:

"Michalak et al. (2005) used a similar objective function for estimating the statistical parameters in the atmospheric inverse problems of surface fluxes."

#### Reference

Michalak, A. M., Hirsch, A., Bruhwiler, L., Gurney, K. R., Peters, W., and Tans, P. P.: Maximum likelihood estimation of covariance parameters for Bayesian atmospheric trace gas surface flux inversions, J. Geophys. Res. [Atmos.], 110, D24107, 10.1029/2005JD005970, 2005.

# **Specific Comments**

**overall** It would be good to list the size of the state vector in various

configurations (with and without concentration).

# **Our reply:**

Thank you for your comment.

The size of the state vector without concentration is 145 (size of scaling factors  $\lambda_i$ ) and the size of the state vector with concentration is 145 (size of scaling factors  $\lambda_i$ ) + 128 × 64 × 28 × 8 × 7 (size of concentration: lon×lat×lev×times/day×days).

We have listed the size of the state vector at the beginning of Section 3 in the revised manuscript:

"The size of the state vector in this study is  $128\times64\times28\times8\times7$  ( $\mathbf{c}_i$ :  $lon\times lat\times lev\times times/day\times days$ ) plus 145 ( $\lambda_i$ )."

**Eq. (1)** Can you justify the 2/3 1/3 split? See later comment for why this might be important.

## **Our reply:**

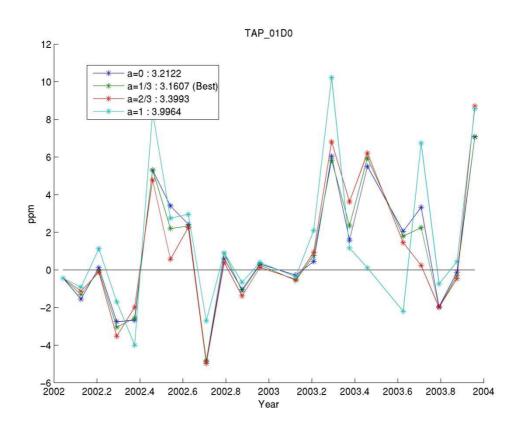
Thank you for your comment.

Actually we choose the (2/3,1/3) split by trial tests. We have tested 7 values of  $\alpha$  in the following formula,

$$\lambda_{t,i}^f = a\lambda_{t-1,i}^a + (1-a) + \sqrt{1-a^2}\zeta_i$$

The forecast CO<sub>2</sub> concentrations in 2002 and 2003 are compared to the measurements in the following steps. First, the monthly means are calculated at each site (for example, Fig. R1 shows the monthly means of

forecast minus measurement at site TAP\_01D0).



**Figure R1.** Residuals of monthly mean forecast minus measurement on site TAP\_01D0 for four cases: a=0,1/3,2/3,1. The numbers in the legend are root mean square errors of monthly means.

Then we can define a root mean square error at individual sites as

$$r_{site} = \sqrt{\frac{1}{M} \sum_{month=1}^{M} r_{site,month}^{2}}$$

where  $r_{site,month}$  is the monthly mean of forecast minus measurement and M is the number of months when there are observations. Finally for all the sites in 2002 and 2003, we use the following relative root mean square error to test different choices of parameter a

$$r_a = \sqrt{\frac{1}{S} \sum_{site=1}^{S} \frac{r_{site}^2}{v_{site}^2}}$$

where  $\left|v_{\mathit{site}}\right|^2$  is the given error variance for each site and S is the

number of sites. The results are listed in Table R1. We can see that in 5 cases a=0,1/6,1/3,1/2,2/3 perform similarly while a=1 performs the worst among all cases. The performance of the case when a=5/6 is between the cases of a=2/3 and a=1. We then chose the median value a=1/3 between a=0 and a=2/3 in our formula. Furthermore, the inflation on forecast error covariance will decrease the impact of different choices of coefficient a.

**Table R1.** Overall relative root mean square error for 7 cases.

	a=0	a=1/6	a=1/3	a=1/2	a=2/3	a=5/6	a=1
$\sqrt{\frac{1}{S} \sum_{site=1}^{S} \frac{r_{site}^2}{v_{site}^2}}$	1.07	1.07	1.06	1.06	1.05	1.12	1.21
(dimensionless)							

**Sec 3.2** We need a little more discussion on the relationship between the iteration of the forecast and analyzed state and the tuning of the inflation parameters. This tuning is set up to ensure that the assumed and actual statistics of departures and innovations are consistent with those assumed in the relevant covariances.

### **Our reply:**

Thank you for your comment.

As discussed in *Tarantola* (2005), we can calculate the  $\chi^2$  statistic of the analysis state for testing the error covariance constructed in this study,

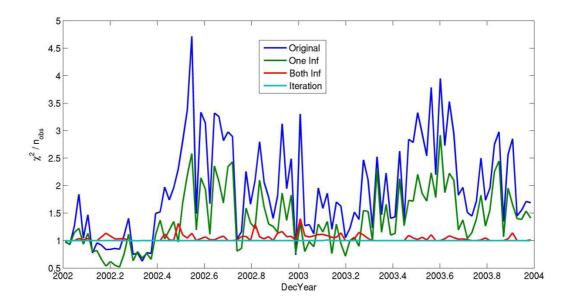
$$\chi_{2,lter}^{2} = \left(\mathbf{y}_{t}^{o} - \mathcal{H}_{t}\left(\mathbf{x}_{t}^{f}\right)\right)^{T} \left(\frac{\theta}{m-1} \mathcal{H}_{t}\left(\widetilde{\mathbf{X}}_{t}^{f}\right) \mathcal{H}_{t}\left(\widetilde{\mathbf{X}}_{t}^{f}\right)^{T} + \mu \mathbf{R}_{t}\right)^{-1} \left(\mathbf{y}_{t}^{o} - \mathcal{H}_{t}\left(\mathbf{x}_{t}^{f}\right)\right)$$

where

$$\widetilde{\mathbf{X}}_{t}^{\mathrm{f}} = \begin{pmatrix} \mathbf{x}_{t,1}^{\mathrm{f}} - \mathbf{x}_{t}^{\mathrm{a}} & \mathbf{x}_{t,2}^{\mathrm{f}} - \mathbf{x}_{t}^{\mathrm{a}} & \cdots & \mathbf{x}_{t,m}^{\mathrm{f}} - \mathbf{x}_{t}^{\mathrm{a}} \end{pmatrix}.$$

and  $\theta$ ,  $\mu$  are the estimated inflation factors for the week associated with  $\widetilde{\mathbf{X}}_t^{\mathrm{f}}$ .  $\mathcal{X}_{2,lter}^2$  should be distributed according to the Chi-square probability density with  $n_{obs}$  degree of freedom, where  $n_{obs}$  is the number of observations within tth week. Since the mean and the variance of  $\mathcal{X}_{2,lter}^2/n_{obs}$  are 1 and  $2/n_{obs}$ , respectively, the value of  $\mathcal{X}_{2,lter}^2/n_{obs}$  should be close to 1.

The Chi-square statistics for the error covariance matrices without using the analysis state can be defined similarly, but with  $\widetilde{\mathbf{X}}_t^{\mathrm{f}}$  replaced by  $\mathbf{X}_t^{\mathrm{f}}$ . They are denoted as  $\mathcal{X}_0^2$ ,  $\mathcal{X}_1^2$  and  $\mathcal{X}_2^2$  for the cases of no inflation, inflation on forecast error only and inflation on both forecast and observation errors, respectively. The closer  $\mathcal{X}_j^2/n_{obs}$ , j=0,1,2 to 1 is, the better the corresponding error statistics.



**Figure R2.**  $\chi^2$  statistic of the analysis state for four estimates of error covariance. "Original" refers to the case without inflations; "One Inf" refers to the case with inflation only on forecast error covariance; "Both Inf" refers to the case with inflations on both forecast and observation error covariance and "Iteration" refers to the case with both inflations and further using analysis to improve forecast error statistics. The closer  $\chi^2/n_{obs}$  is to 1, the better the corresponding error estimates.

For validating the construction of error statistics used in this study, the weekly time series of  $\chi^2_{2,ler}/n_{obs}$  from 2002 to 2003 is shown in Fig. R2. It is remarkably close to 1. The weekly time series of  $\chi^2_0/n_{obs}$ ,  $\chi^2_1/n_{obs}$  and  $\chi^2_2/n_{obs}$  for the cases of no inflation, inflation on forecast error only and inflation on both forecast and observation errors are also shown in Fig. R2. All of them are not as close to 1 as that of  $\chi^2_{2,lter}/n_{obs}$ . This indicates that the construction of error statistics using the analysis state iteratively is effective for correctly estimating the error statistics. Figure R2 also shows that  $\chi^2_2/n_{obs}$  is closer to 1 than  $\chi^2_1/n_{obs}$  is, and both are closer to 1 than  $\chi^2_0/n_{obs}$  is. This suggests that the inflation on forecast

error and observation error are also both effective in improving the estimation of error statistics.

The above discussions have been added to the revised manuscript.

#### Reference.

Tarantola, A.: Inverse Problem Theory and Methods for Model Parameter Estimation, Other Titles in Applied Mathematics, Society for Industrial and Applied Mathematics, 348 pp., 2005.

I'm not quite sure what consistency is enforced by the iteration in Sec 2.2 and am a little concerned that the observations might be implicitly used twice, once via the analyzed state now used to describe the forecast uncertainty then again in the update step. This probably reflects limited understanding on my part but I doubt I am alone.

## **Our reply:**

Now we have given some proof of the effectiveness of using analysis to improve the estimation of forecast error covariance by Chi-square test. On the other hand, theoretically the basic assumption of EnKF assimilation is that the forecast and observation are statistically independent. In our iterative scheme, the ensemble forecast is always the same, that is, using observations to estimate the forecast uncertainty do not change the ensemble forecast, so this basic assumption is not violated. Furthermore, in all existing schemes for adaptive estimation of the inflation factor, observations are also used to estimate the forecast

uncertainty since it is the forecast uncertainty being inflated (e.g. *Anderson* (2007), *Li et al.* (2009), *Michalak et al.* (2005), *Miyoshi* (2011), *Wang and Bishop* (2003)). Therefore, we feel that using observations to estimate the forecast uncertainty is justified.

#### References.

Anderson, J. L.: An adaptive covariance inflation error correction algorithm for ensemble filters, Tellus Ser. A-dynamic Meteorology and Oceanography, 59(2), 210--224, doi:10.1111/j.1600-0870.2006.00216.x, 2007.

Li, H., E. Kalnay, and T. Miyoshi: Simultaneous estimation of covariance inflation and observation errors within an ensemble Kalman filter, Q. J. R. Meteorolog. Soc., 135(639), 523--533, doi:10.1002/qj.371, 2009.

Michalak, A. M., Hirsch, A., Bruhwiler, L., Gurney, K. R., Peters, W., and Tans, P. P.: Maximum likelihood estimation of covariance parameters for Bayesian atmospheric trace gas surface flux inversions, J. Geophys. Res. [Atmos.], 110, D24107, 10.1029/2005JD005970, 2005.

Miyoshi, T.: The Gaussian approach to adaptive covariance inflation and its implementation with the local ensemble transform Kalman filter, Mon. Weather Rev., 139(5), 1519—1535, 2011.

Wang, X., and C. H. Bishop: A Comparison of Breeding and Ensemble Transform Kalman Filter Ensemble Forecast Schemes, J. Atmos. Sci., 60(9), 1140--1158, doi:10.1175/1520-0469(2003)060<1140:ACOBAE>2.0.CO;2, 2003.

P6530 it's a fascinating idea that by hugely increasing the size of the state vector (including concentration) you can actually reduce the computational cost. Shouldn't this be compensated by requiring different ensemble sizes to span the much larger space?

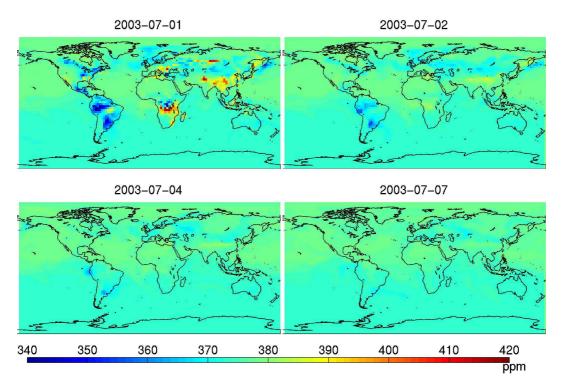
#### **Our reply:**

Thank you for your comments.

We fully agree with you that if we increase hugely the size of the state vector, we have to increase the ensemble sizes.

However, since the size of scaling factor vector  $\lambda_i$  is 145 in this study, the degrees of freedom of surface flux sets are less than 145.

On the other hand, the concentrations mix rapidly by diffusion in one week. An intuitional example is given in Fig. R3. We started from one modeled concentration field in July  $1^{\rm st}$ , 2003, and forecasted the concentration field in the following week without any carbon fluxes at land surface (i.e. zero boundary conditions). In this way the diffusion and advection of  $CO_2$  existing in atmosphere at July  $1^{\rm st}$ , 2003, can be investigated. We have plotted the lowest vertical model level since it is most strongly influenced by previous carbon fluxes and thus has largest varibilities at the starting time. It can be seen that after one week the concentration field becomes very smooth. Therefore, the atmospheric  $CO_2$  concentration is mixed rapidly with time and it does not have as large degree of freedom as the size itself.



**Figure R3**. Forecast of concentration field in the lowest vertical model level in one week without carbon fluxes as boundary conditions.

Actually we determined the size of ensemble (150) by experiments. The difference of the assimilated carbon budgets in 2002 is within 10% and the patterns are very similar when we use different ensemble sizes of 150 and 200.

For all above reasons we chose 150 as the default ensemble size in GCAS-EK.

P6531 The bias in the simulation after analysis could be disturbing if it represents a miscalculation of the trend in concentration. Could you plot this bias as a function of time? If there is an error in the concentration trend this would suggest an error in the long-term fluxes.

This is worth discussing since it's always seemed possible in these weak-constraint formulations that we might not match the long-term growth rate.

### **Our reply:**

Thank you for your comments.

Following your advice, we calculated the long-term growth rate in different cases. Atmospheric CO<sub>2</sub> concentration is generated using the sequential forecast of CO<sub>2</sub> concentration with the prior and optimized carbon fluxes, respectively, from 2002 to 2008. The annual mean growth rate with optimized flux (2.17 ppm yr<sup>-1</sup>) is much closer to observations (2.14 ppm yr<sup>-1</sup>) than that with prior flux (3.13 ppm yr<sup>-1</sup>), indicating that we have a good match with the long-term growth rate after optimization. The time series of the bias look similar to the scatter plot in Fig. 6 in the revised manuscript.

We have added the analysis of the long-term growth rates in the revised manuscript.

Sec 6.2] Some of the concern over low variability in may be explained by Eq. 1. The division by 3 should have the effect of strongly smoothing.

What would happen if you replaced Eq. 1 with a pure random walk model?

### **Our reply:**

Thank you for your comments.

Some comparisons between Eq. 1 (a=1/3) and a pure random walk model (a=0) can be found in our reply to Specific Comment 2. The overall relative root mean square errors of forecasted  $CO_2$  observations are very close. The estimated annual carbon budget in 2002 and 2003 with the model with a=1/3 is 15% more on average than that with the model with a=0.

However these two models perform differently at individual sites. It can be found in Fig. R4 that which model performs better at each observation site. The sites at which the a=1/3 model performs better are mostly located in or closely to land areas. Since we focus on the optimization of ecosystem carbon fluxes, we prefer to use the strong smoothing model with a=1/3.

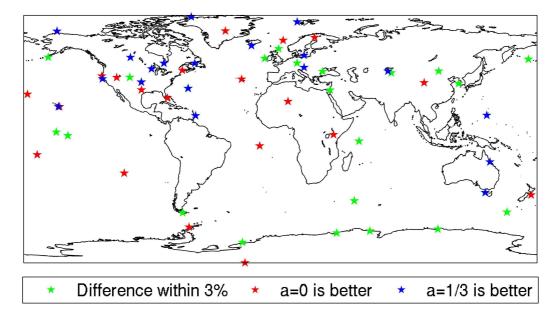


Figure R4. Performance of model a=0 and a=1/3 at different sites. The green stars indicate that these two models have almost equal performance. The red stars indicates that the model with a=0 performs much better at these sites than the model with a=1/3. The blue stars indicates that the model with a=1/3 performs much

better at these sites than the model with a=0.

# A Global Carbon Assimilation System using a modified

1

2

3

20

# 域代码已更改 域代码已更改 域代码已更改

# EnKF assimilation methodEnsemble Kalman filter

Shupeng Zhang<sup>a,b</sup>, Xiaogu Zheng<sup>a,b\*</sup>, Jing M. Chen<sup>b,c,d</sup>, Zhuoqi Chen<sup>a,b</sup>, Bo Dan<sup>a,b</sup>, 4 Xue Yi<sup>a,b</sup>, Liqun Wang<sup>e</sup> and Guocan Wu<sup>a,b</sup> 5 6 7 <sup>a</sup>College of Global Change and Earth System Science, 8 Beijing Normal University, Beijing, China 9 <sup>b</sup>Joint Center for Global Change Studies, Beijing, China 10 <sup>c</sup>Department of Geography, University of Toronto, Toronto, Canada 11 <sup>d</sup>International Institute for Earth System Science, 12 Nanjing University, Nanjing, China 13 <sup>e</sup>Department of Statistics, University of Manitoba, Winnipeg, Canada 14 15 16 \*Correspondence to: X. Zheng, College of Global Change and Earth System Science, 17 Beijing Normal University, #19 Xinjiekouwai St, Beijing, 100875 China, Email: 18 x.zheng@bnu.edu.cn 19

### Abstract

3

1

2

A Global Carbon Assimilation System based on the Ensemble Kalman filter 4 (GCAS-EK) is developed for assimilating atmospheric CO<sub>2</sub> abundance—data into an 5 ecosystem model to simultaneously estimate the surface carbon fluxes and 6 7 atmospheric CO<sub>2</sub> distribution. This assimilation approach is similar to CarbonTrackerbased on the ensemble Kalman filter (EnKF), but with several new 8 developments, including inclusion of atmospheric CO2 concentration in state vectors, 9 10 using the Ensemble Kalman filter (EnKF) with one-week assimilation windows, using analysis states to iteratively estimate ensemble forecast errors, and a maximum 11 likelihood estimation of the inflation factors of the forecast and observation errors. 12 The proposed assimilation approach is tested in observing system simulation 13 experiments and then used to estimate the terrestrial ecosystem carbon fluxes and 14 atmospheric CO<sub>2</sub> distributions from 2002 to 2008. The results showed that this 15 assimilation approach can effectively reduce the biases and uncertainties of the carbon 16 fluxes simulated by the ecosystem model. 17

18

19

- Keywords: Data assimilation, Ensemble Kalman filter, Ecosystem modeling,
- 20 Atmospheric transport, CO<sub>2</sub> mole fraction, Surface carbon fluxes

### 1 Introduction

3

7

10

12

15

16

17

18

19

20

21

22

23

24

25

1

2

4 The carbon dioxide concentration in the atmosphere plays an essential role in the

5 study of global change for its potential to warm up the atmosphere and the surface. A

6 better estimation of carbon fluxes over global ecosystems would help better

understand each nation's contribution to-the global warming and improve the global

8 warming science.

In the past decade, many efforts have been made to estimate the surface  $CO_2$ 

fluxes using both atmosphere-based top-down and land-based bottom-up methods.

11 CarbonTracker (Peters et al., 2005; Peters et al., 2007) may be one of the most

advanced among these efforts. It uses an ensemble square root filter to assimilate

13 atmospheric  $CO_2$  mole fractions into an ecosystem model coupled with an

14 atmospheric transport model.

The model state vectors in CarbonTracker are carbon fluxes only within 5 weeks. However, the observed CO<sub>2</sub> consists of both initial state of atmosphere CO<sub>2</sub> and recently released carbon fluxes, so including CO<sub>2</sub> concentration in the state vectors should improve the estimation of initial atmosphere CO<sub>2</sub> (Miyazaki et al., 2011). This could lead to further improvement of carbon flux estimation. Kang et al. (2011) Kang et al. (2011);(Kang et al., 2012) and Liu et al. (2012) also added CO<sub>2</sub> concentrations to the state vectors due to their strong correlations with weather variables that are simultaneously assimilated. argued that the state vectors should also include atmospheric CO<sub>2</sub> concentration, because the observed CO<sub>2</sub> consists of both existing atmosphere CO<sub>2</sub> and recently released earbon fluxes, so including CO<sub>2</sub> concentration

域代码已更改

in the state vectors should improve the estimation of carbon fluxes. However, their

efforts mainly focus on studying the performance of the assimilation methodology and observation settings by using idealized models only, not on assimilating real observations.

The length of the assimilation window in CarbonTracker is 5 weeks. This would include CO<sub>2</sub> observations far from the analysis time. However this may not necessarily improve the flux analysis compared to an instantaneous analysis due to the attenuation of the detailed information as discussed by Enting (2002). A shorter assimilation window reduces the attenuation of observed CO<sub>2</sub> information, because the analysis system can use near-surface CO<sub>2</sub> observations before the transport of CO<sub>2</sub> blurs out the essential information of near-surface CO<sub>2</sub> forcing (Kang et al., 2012).

It is well known that correct estimation of the forecast error statistics is crucial for the accuracy of any data assimilation algorithm. In all existing EnKF assimilations for estimating carbon fluxes, the ensemble forecast errors are estimated by the difference of perturbed forecasts minusand their ensemble mean. However, the definition of the The perturbed forecast errors—is are defined as the perturbed forecast states minus the true state. Motivated by the fact that the analysis state is a better estimate of the true state than the forecast state, Wu et al. (2013) proposed a new estimator for the perturbed forecast errors by using the difference between the perturbed forecast states minus—and the analysis state. Moreover, they used a simulation study to demonstrated through a simulation study that the new estimator can lead to better assimilations for models with large errors. Since the model—errors of ecosystem models are generally large, the new estimation of the perturbed forecast errors is potentially useful to improve EnKF assimilation for estimating carbon fluxes.

Besides forecast errors, the observation errors need also be accurately estimated. In the majority of schemes for estimating carbon fluxes, including CarbonTracker, the

observation error variances are not estimated but empirically assigned. The quality of 1 the estimation of observation error variances critically depends on whether the 2 forecast error covariance matrix is appropriately estimated or not (Desroziers et al., 3 2005). However, appropriate estimation of the forecast error covariance matrix is a 4 5 challenge in real applications. In this paper, we propose several modifications to the conventional EnKF for 6 7 assimilating atmospheric CO<sub>2</sub> observations into ecosystem models. Firstly, the model state is set as a combination of contains both the surface carbon fluxes and 8 atmospheric CO2 concentration as suggested by Miyazaki et al. (2011). Kang et al. 9 (2011) and Liu et al. (2012) and. Secondly, the analysis state is used to adaptively 10 11 estimate forecast errors as suggested by Wu et al. (2013) and Zheng et al. (2013)-, and Thirdly, both forecast and observation errors are inflated as suggested by-Liang et al. 12 13 (2012) Liang et al (2012). Finally, the one-week assimilation window is tested against longer windows. This modified EnKF is used to assimilate real CO<sub>2</sub> concentration 14 data into the Boreal Ecosystem Productivity Simulator (BEPS, Chen et al., 1999; Liu 15 et al., 1999; Mo et al., 2008) for estimating the real world terrestrial carbon fluxes 16 17 with 3 hourly and 1°×1° resolution from 2002 to 2008. 18 This paper consists of  $\frac{7}{6}$  sections. The models and data used in this study are 19 introduced in Section 2, while the methodology is described in Section 3. Section 4 presents the validations of the new methodologies using the real observing system. 20 simulation experiment results. A real data application of the proposed methodology is 21 presented in Section 5. Conclusions and discussions are given in Sections 6. and 7 22

25 2 Models and Data

respectively.

23

### 2 2.1 Surface carbon flux models

1

3

8

9

10

11

12

13

14

15

16

17

18

19

20

21

22

23

24

25

The surface carbon fluxes mainly arise from fossil fuel combustion, vegetation fire, oceanic <a href="mailto:uptake-exchange">uptake-exchange</a> and biosphere. In this study, only the surface carbon fluxes from biosphere are simulated using BEPS, <a href="mailto:while">while</a> the rests are taken from datasets of CarbonTracker 2011 (<a href="http://www.esrl.noaa.gov/gmd/ccgg/carbontracker/">http://www.esrl.noaa.gov/gmd/ccgg/carbontracker/</a>).

BEPS is a process-based ecosystem model mainly developed to simulate forest ecosystem carbon budgets (Chen et al., 1999; Ju et al., 2006; Liu et al., 1999). For many reasons, such as including the complexity of ecosystem processes, spatial-temporal variabilities, and representative errors, parameters in process-based models often do not represent their true values when these models are used to calculate carbon budgets over large areas and or for long time periods (Mo et al., 2008). Errors in these parameters lead to biases of in model results (Other uncertainties, such as lack of knowledge on historical land-use change and land management, also have influence on model results). In this study, we try to reduce biases of in the BEPS\_-simulated carbon fluxes by incorporating atmospheric CO<sub>2</sub> concentration measurements with data assimilation methods. The prior carbon fluxes simulated by BEPS are at a spatial resolution of 1°×1° and for every 3-one hours. On each model grid, BEPS calculates carbon fluxes of 6 different ecosystem plant function types and outputs the sum of them through weighting the fluxes against areal fractions of the ecosystem-plant function types. Figure 1 shows the ecosystem-plant <u>function</u> types with the largest weight on each grid.

The vegetation fire flux is taken from CarbonTracker 2011 dataset, which is modeled using the Carnegie-Ames Stanford Approach (CASA) biosphere model

(Potter et al., 1993) based on the Global Fire Emission Database (GFED) (van der 1 Werf et al., 2006). 2 The oceanic CO<sub>2</sub> flux is taken from CarbonTracker 2011 optimized results, 3 whose a priori estimates are based on two different datasets: namely ocean inversion 4 flux result (Jacobson et al., 2007) and pCO<sub>2</sub>-Clim prior derived from the climatology 5 6 of seawater pCO<sub>2</sub> (Takahashi et al., 2009). 7 The fossil fuel combustion estimate is the dataset preprocessed by CarbonTracker 2011 from the global total fossil fuel emission of the Carbon Dioxide Information and 8 Analysis Center (CDIAC) (Boden et al., 2011) and the "ODIAC" emission dataset 9 (Oda and Maksyutov, 2011). 10 11 2.2 Atmospheric transport model 12 13 The global chemical transport Model for OZone And Related chemical Tracers 14 (MOZART, Emmons et al., 2010) is used as the atmospheric transport model. In this 15 study, MOZART is run at a horizontal resolution of approximately 2.8°×2.8° with 16 28 vertical levels. The forcing meteorology is from NCAR reanalysis of the National 17 Centers for Environmental Prediction (NCEP) forecasts (Kalnay et al., 1996; Kistler et 18 al., 2001). Since CO<sub>2</sub> is chemically inert in atmosphere, we turn off all the 19 chemicalstry processes and leave only transport of CO2 by atmospheric motions. 20 Given the atmospheric CO<sub>2</sub> concentration in the previous week and the surface carbon 21

concentration within the current week.

2.3 Observation

22

25

fluxes in the current week, MOZART is used to forecast gridded atmospheric CO2

1	
2	The atmospheric CO <sub>2</sub> concentration measurements collected and preprocessed by
3	CarbonTrackerObservation Package (ObsPack) Data Product (Masarie et al., 2014)
4	are used in this study (Product Version:
5	obspack_co2_1_CARBONTRACKER_CT2013_2014-05-08). It reflects the
6	variability of the total surface carbon fluxes (i.e. fossil fuel combustion, vegetation
7	fire, oceanic uptake and biosphere) as well as inter exchange among the CO2 existing
8	in the atmosphere. The CO <sub>2</sub> dataset released on CarbonTracker's website
9	(http://www.esrl.noaa.gov/gmd/ccgg/carbontracker/) The selected CO <sub>2</sub> measurements
10	on 92 sites includes observations of two main types: the measurements of air samples
11	at surface sites and in situ quasi-continuous CO <sub>2</sub> time series from towers. Since some
12	stations have multiple observations within a week, Onon average there are about 140
13	observations in every week during 2000 and 2010 2008. Six laboratories (NOAA)
14	Global Monitoring Division, Commonwealth Scientific and Industrial Research
15	Organization, National Center For Atmospheric Research, Environment Canada,
16	Lawrence Berkeley National Laboratory and Instituto de Pesquisas Energeticas e
17	Nucleares) provided these measurements and information of observation sites used in
18	this study is listed in Table 1. CO <sub>2</sub> concentration measurements reflect the variability
19	of the total surface carbon fluxes (i.e. fossil fuel combustion, vegetation fire, oceanic
20	uptake and biosphere) as well as inter-exchange among CO <sub>2</sub> air mass in the initial
21	atmosphere.
22	The observation error variances dataset is also released on CarbonTracker's
23	websiteare also provided in
24	obspack_co2_1_CARBONTRACKER_CT2013_2014-05-08. They were subjectively

chosen and manually tuned to fit into their models specific atmospheric transport

models and observations (Peters et al., 2005; Peters et al., 2007). The observation sites 1 were divided into six categories, each with their own assigned observation errors (see 2 the document of CarbonTracker for details). These observation error variances Since 3 4 these values depend on the atmospheric transport model used in a carbon data assimilation system, they are just used as prior values in our system for this study and 5 are will be adaptively adjusted with the proposed assimilation scheme. 6 7 Methodology 8 9 Within tth week, let  $\mathbf{c}_t$  be a set of gridded atmospheric CO<sub>2</sub> concentrations every 3 10 hours,  $\mathbf{f}_t$  be the set of prior carbon fluxes every 3 hours, and  $\lambda_t$  be a set of factors 11 12 defined as constants on areas and within a week for adjusting  $f_{i}$ . Then, the model state is defined as  $\mathbf{x}_{t} = (\mathbf{c}_{t}^{\mathrm{T}}, \boldsymbol{\lambda}_{t}^{\mathrm{T}})^{\mathrm{T}}$ . In this study, only land surface carbon fluxes need 13 to be adjusted. The partition of the adjustment factors (i.e.  $\lambda_t$ ) is based on 11 14 TransCom regions (Gurney et al., 2004) and 19 Olson ecosystem types, as in 15 CarbonTracker. Thus the size of the state vector in this study is 128×64×28×8×7 (c; 16  $lon \times lat \times lev \times times/day \times days)$  plus 145 ( $\lambda_t$ ). We refer to this data assimilation scheme 17 as Global Carbon Assimilation System using Ensemble Kalman filter (GCAS-EK). 18 19 3.1 EnKF with error inflations 20 21

域代码已更改

Using the notations of Ide et al. (1997), the first EnKF algorithm used in this study

consists of the following three main steps:

22

- 1 1) Forecast step
- 2 The perturbed forecast states are estimated as

$$\lambda_{t,i}^{f} = \frac{2}{3} + \frac{1}{3} \lambda_{t-1,i}^{a} + \xi_{t,i}$$
 (1)

$$\mathbf{c}_{t,i}^{f} = G\left(\mathbf{c}_{t-1,i}^{a}, \boldsymbol{\lambda}_{t,i}^{f}\right) \tag{2}$$

- 5 where i represents an ensemble member,  $\xi_{t,i}$  are vectors sampled from a
- 6 distribution with mean <u>Ozero</u> and a given covariance matrix (taken from prior
- 7 covariance structure in CarbonTracker, see the document of CarbonTracker and
- 8 (Peters et al., 2005; Peters et al., 2007)), and G is the atmospheric transport operator
- 9 which maps  $\mathbf{c}_{t-1}$  and the  $\lambda_t$ -adjusted  $\mathbf{f}_t$  onto gridded CO<sub>2</sub> concentration. Then the
- 10 forecast state is estimated as

11 
$$\mathbf{x}_{t}^{f} = \frac{1}{m} \sum_{i=1}^{m} \mathbf{x}_{t,i}^{f}$$
, (3)

- where m is the ensemble size.
- 13 2) Error step
- The ensemble forecast errors and the observation error covariance matrix are
- 15 estimated as  $\sqrt{\theta_t} \mathbf{X}_t^f$  and  $\mu_t \mathbf{R}_t$  respectively, where

$$\mathbf{X}_{t}^{f} = \begin{pmatrix} \mathbf{x}_{t,1}^{f} - \mathbf{x}_{t}^{f} & \mathbf{x}_{t,2}^{f} - \mathbf{x}_{t}^{f} & \cdots & \mathbf{x}_{t,m}^{f} - \mathbf{x}_{t}^{f} \end{pmatrix}, \tag{4}$$

- and  $\mathbf{R}_t$  is the <u>prescribed</u> observation error <u>co</u>variance matrix <u>for CarbonTracker</u>.  $\theta_t$
- and  $\mu_t$  are the inflation factors (of the forecast error and the observation error
- respectively) which are estimated by minimizing the following objective function
- 20 (Liang et al., 2012; Zheng, 2009):

$$-2L_{t}(\boldsymbol{\theta}, \boldsymbol{\mu}) = \ln \left\{ \det \left( \frac{\boldsymbol{\theta}}{m-1} \mathcal{H}_{t} \left( \mathbf{X}_{t}^{f} \right) \mathcal{H}_{t} \left( \mathbf{X}_{t}^{f} \right)^{T} + \boldsymbol{\mu} \mathbf{R}_{t} \right) \right\}$$

$$+ \left( \mathbf{y}_{t}^{o} - \mathcal{H}_{t} \left( \mathbf{x}_{t}^{f} \right) \right)^{T} \left( \frac{\boldsymbol{\theta}}{m-1} \mathcal{H}_{t} \left( \mathbf{X}_{t}^{f} \right) \left( \mathcal{H}_{t} \left( \mathbf{X}_{t}^{f} \right) \right)^{T} + \boldsymbol{\mu} \mathbf{R}_{t} \right)^{-1} \left( \mathbf{y}_{t}^{o} - \mathcal{H}_{t} \left( \mathbf{x}_{t}^{f} \right) \right)$$

$$(5)$$

- where  $\mathbf{y}_{t}^{\circ}$  is the vector of atmospheric CO<sub>2</sub> concentration measurements,  $\mathcal{H}_{t}$  is a
- 3 linear observation operator, which interpolates gridded CO<sub>2</sub> concentrations at
- 4 observation times and locations. Michalak et al. (2005) used a similar objective
- 5 function for estimating the statistical parameters in the atmospheric inverse problems
- 6 of surface fluxes.
- 7 3) Analysis step
- 8 The perturbed analysis states are estimated as

$$\mathbf{x}_{t,i}^{a} = \mathbf{x}_{t,i}^{f} + \sqrt{\theta_{t}} \mathbf{X}_{t}^{f} \left[ (m-1)\mathbf{I} + \mathcal{H}_{t} \left( \sqrt{\theta_{t}} \mathbf{X}_{t}^{f} \right)^{T} \left( \mu_{t} \mathbf{R}_{t} \right)^{-1} \mathcal{H}_{t} \left( \sqrt{\theta_{t}} \mathbf{X}_{t}^{f} \right) \right]^{-1}$$

$$\left( \mathcal{H}_{t} \left( \sqrt{\theta_{t}} \mathbf{X}_{t}^{f} \right) \right)^{T} \left( \mu_{t} \mathbf{R}_{t} \right)^{-1} \left( \mathbf{y}_{t}^{o} - \mathcal{H}_{t} \left( \mathbf{x}_{t,i}^{f} \right) + \varepsilon_{t,i} \right)$$

- where  $\varepsilon_{t,i}$  is a normal random variable with mean zero and covariance matrix  $\mu_t \mathbf{R}_t$
- 12 (Burgers et al., 1998). The analysis state  $\mathbf{x}_{t}^{a}$  is estimated as

$$\mathbf{x}_{t}^{\mathbf{a}} = \frac{1}{m} \sum_{i=1}^{m} \mathbf{x}_{t,i}^{\mathbf{a}} \tag{7}$$

- Finally, set t = t + 1 and return to step (1) for the assimilation at next time step.
- The assimilated surface carbon fluxes are from all sources because the observed
- 16 CO<sub>2</sub> concentrations are arising arise from all sources. Then, the surface carbon fluxes
- from the biosphere are estimated by the assimilated total carbon fluxes minus carbon
- 18 fluxes from other sources supplied by the forcing data.

20 3.2 Constructing error statistics using analysis

Let  $\mathbf{x}_{t}^{t}$  be the true state. The<u>n the</u> ensemble forecast error should be defined as  $\mathbf{x}_{t,i}^{\mathrm{f}} - \mathbf{x}_{t}^{\mathrm{t}}$ . However,  $\mathbf{x}_{t}^{\mathrm{t}}$  is estimated by  $\mathbf{x}_{t}^{\mathrm{f}}$  in Eq.(4). Since  $\mathbf{x}_{t}^{\mathrm{a}}$  is derived by assimilating observations into the model, it should be is a better estimate of  $\mathbf{x}_t^t$  than  $\mathbf{x}_{t}^{\mathrm{f}}$ , especially when the model error is large (Wu et al., 2013). Therefore after the analysis step 3) in Section 3.1, it is suggested to return to the error step 2), and substitute  $\mathbf{x}_t^{\mathrm{f}}$  in Eq.(4) by  $\mathbf{x}_t^{\mathrm{a}}$ . This procedure is repeated until the corresponding objective function (Eq.(5)) converges (Wu et al., 2013; Zheng et al., 2013). In this study, the iteration is stopped whenif the difference between the minima of  $-2L_t(\theta,\mu)$  at *n*-th and *n*+1th iterations is less one 1., then the iteration is stopped. A 

flowchart of the proposed assimilation scheme in this study is shown in Fig. 2.

### 3.3 Removing carbon mass imbalance

In this study, the background  $CO_2$  concentration field at the beginning of a week is the analysis state at the end of the previous week. It is then updated using the observations within the week, so the estimated  $CO_2$  concentration at the beginning of the week is different from that at the end of the previous week. This results in inexact carbon mass balance. To remove this imbalance, a corrected atmospheric  $CO_2$  concentration is generated using the sequential forecast of  $CO_2$  concentration with the optimized carbon fluxes from the very beginning of the entire assimilation period. The corrected  $CO_2$  concentration is denoted by  $\mathbf{c}_i^{ca}$ .

## 3.4 Validation statistics

1

3

4

6

7

8

9

10

11

12

13

14

15

16

17

18

19

20

2 Chi-square statistics (Tarantola, 2005) are used to test the error covariances

constructed in this study. For the tth week, it is defined as

域代码已更改域代码已更改

5 where

 $\underline{\mathbf{X}}_{t}^{f} = (\mathbf{x}_{t,1}^{f} - \mathbf{x}_{t}^{a} \quad \mathbf{x}_{t,2}^{f} - \mathbf{x}_{t}^{a} \quad \cdots \quad \mathbf{x}_{t,m}^{f} - \mathbf{x}_{t}^{a})$  (9)

域代码已更改 域代码已更改

and  $\theta$ ,  $\mu$  are the estimated inflation factors for the week. If the forecast and

域代码已更改 域代码已更改

域代码已更改

域代码已更改

observation error covariance matrix are correctly estimated,  $\chi^2_{2,lter}$  follows a

<u>Chi-square distribution with  $n_{obs}$  degrees of freedom, where  $n_{obs}$  is the number of</u>

observations within th week. Since the mean and the variance of  $\chi^2_{2,lter}/n_{obs}$  are 1

and  $2/n_{obs}$  respectively, the value of  $\chi^2_{2,lter}/n_{obs}$  should be close to 1.

The Chi-square statistics for the error covariance matrices without using the

analysis state can be defined similarly to Eq. (8), but with  $\widetilde{\mathbf{X}}_{t}^{\mathrm{f}}$  replaced by  $\mathbf{X}_{t}^{\mathrm{f}}$ .

They are denoted as  $\chi_0^2 - \chi_1^2$  and  $\chi_2^2$  for the cases of no inflation, inflation on

forecast error only and inflation on both forecast and observation errors, respectively.

The closer  $\chi_j^2/n_{obs}$ , j = 0,1,2 to 1 is, the better the corresponding error statistics.

The root mean square error (RMSE) of estimated CO<sub>2</sub> observations is defined as

$$-\sqrt{\frac{1}{L}\sum_{i,l}(y_{i}^{ca}(l)-y_{i}^{o}(l))^{2}}$$
 (10)

where  $y_i^{ca}(l)$  is generated by interpolating  $\mathbf{e}_t^{ca}$  to the observation site l and time i,

and L is the total number of the  $CO_2$  concentration observations during the entire

assimilation period. The smaller RMSE means better assimilation scheme.

2

3

4

6

7

8

9

10

12

13

14

15

1

In ideal experiments where the "truth" is known, we can calculate the root mean square error (RMSE) of the model states. RMSE of carbon fluxes is defined as

5 defined a

$$\sigma(k) = \sqrt{\frac{1}{T} \sum_{t=1}^{T} \left( f_t(k) - f_t^{t}(k) \right)^2}$$
(8)

where T -stands for the total period of the assimilation,  $f_t(k)$  is an average of

fluxes in the &th TransCom region (Gurney et al., 2004) and &th 3 hour period,

while  $-f_t^{t}$  is the corresponding "truth". The spread is defined as,

$$\frac{1}{\sqrt{T(m-1)}} \sum_{t=1}^{T} \sum_{j=1}^{m} \left( f_{t,j}(k) - \frac{1}{m} \sum_{i=1}^{m} f_{t,i}(k) \right)^{2}$$
 (9)

11 where  $f_{i,j}(k)$  is the jth member of ensemble fluxes in the kth TransCom region. If

all the members of ensemble analysis states have the same distribution as the "truth",

then estimated RMSE and spread should be close.

The RMSE of CO<sub>2</sub> concentrations at -tth time is defined as

$$\frac{1}{\sqrt{L}} \sum_{l=1}^{L} \left( y_{t}(l) - y_{t}^{t}(l) \right)^{2} \tag{10}$$

16 where  $y_i(l)$  is the CO<sub>2</sub>-concentration value at -lth location and  $-y_i^t(l)$  is the

corresponding "truth".

18

17

19

4 Simulation study Discussions on methodology

21

1	4.1 Error covariance statistics
2	
3	To validate the construction of error statistics used in this study, we plot the weekly
4	time series of $\chi^2_{2,lter}/n_{obs}$ (Eq. 8) from 2002 to 2003 in Fig. 3, which shows that the
5	values are remarkably close to 1. In contrast, the weekly time series of $\chi_0^2/n_{obs}$
6	$\chi_1^2/n_{obs}$ and $\chi_2^2/n_{obs}$ (for the cases of no inflation, inflation on forecast error only
7	and inflation on both forecast and observation errors) are not as close to 1 as
8	$\chi_{2,lter}^2/n_{obs}$ . This indicates that the construction of error statistics using the analysis
9	state iteratively (Section 3.2) is effective for correctly estimating the error statistics.
10	Fig. 3 also shows that $\chi_2^2/n_{obs}$ is closer to 1 than $\chi_1^2/n_{obs}$ is, and both are
11	closer to 1 than $\chi_0^2/n_{obs}$ is. This suggests that the inflations on forecast error and
12	observation error are also both effective in improving the estimation of error statistics.
13	
14	4.2 Inclusion of CO <sub>2</sub> concentration in state vectors
15	
16	In this study, the CO <sub>2</sub> concentration is included in state vectors. The benefit of this
17	inclusion needs to be tested against the traditional approach without this inclusion.
18	This issue is studied with the one-week assimilation window.
19	For this purpose we design a comparative experiment as follows. In every week,
20	the CO <sub>2</sub> concentration (i.e. <u>c</u> ) is not updated (Eq. 6). Instead the analysis CO <sub>2</sub>
21	concentration is derived by sequentially predicting atmospheric CO <sub>2</sub> concentration
22	forced by the updated flux within the week. The carbon mass is automatically
22	halanced in this experiment. The results show that RMSF of the analysis CO <sub>2</sub>

concentration observations (Eq. 10) is 8.5% larger than that of the corrected analysis

CO<sub>2</sub> concentration described in Section 3.3. This suggests that inclusion of CO<sub>2</sub>

concentration in state vectors can significantly alter the CO<sub>2</sub> mass balance and may

have advantage in optimizing the surface CO<sub>2</sub> flux.

If the CO<sub>2</sub> concentration is not included in state vectors, the analysis CO<sub>2</sub> concentration at the beginning of each week is just the analysis CO<sub>2</sub> concentration at the end of the previous week, so the CO<sub>2</sub> concentration observations within the current week are not used to optimize the CO<sub>2</sub> concentration at the beginning of each week. However, when the CO<sub>2</sub> concentration is included in state vectors, all the observations within the current week and the previous weeks are used to estimate the CO<sub>2</sub> concentration at the beginning of the current week. So the CO<sub>2</sub> concentration at the beginning of each week estimated by inclusion of CO<sub>2</sub> concentration in state vectors could be more accurate than estimated without inclusion. Therefore, the estimated flux associated with the updated CO<sub>2</sub> concentration at the beginning of the current week should have better quality. This is demonstrated by smaller RMSE (Eq. 10) with the inclusion than that without the inclusion.

### 4.3 Length of assimilation window

Different lengths of the assimilation window are used in various systems (5 weeks in CarbonTracker, 3 and 7 days in Miyazaki et al. (2011) and 6 hours in Kang et al. (2012)). We choose the one-week assimilation window in our methodology for the following reasons. First, since most surface stations only have weekly observations, we need at least one week data to cover the globe. Second, beyond one week the errors of the atmospheric transport model may be significant, and they are very

difficult to quantify. Third, the detailed information of observations may be attenuated with time by atmospheric diffusion and advection (Enting, 2002).

For comparison to longer assimilation windows, the following alternative experiments with moving assimilation windows were carried out. In the first alternative experiment, the length of the moving window is set to be two weeks while the forecast time step is still one week. The CO<sub>2</sub> concentration observation system is still the same as that described in Section 3, but is used to update the global carbon flux and the atmospheric CO<sub>2</sub> concentration within the current week and the previous week. This procedure is similar to Eq. 6, while the ensemble forecast state of the first week in the assimilation window is set as its ensemble analysis state at previous assimilation time step. Therefore carbon fluxes and CO<sub>2</sub> concentration every week are optimized twice with the observations in the current week and the next week. The corrected analysis of CO<sub>2</sub> concentration is also retrieved from reruning the atmospheric transport model as described in Section 3.3. The second alternative experiment is similar to the first one, but with the three-week moving window.

The linear trends for the observations, the estimates with one-week, two-week and three-week moving windows are 2.14ppm yr<sup>-1</sup>, 2.17 ppm yr<sup>-1</sup>, 1.59 ppm yr<sup>-1</sup>, and 1.13 ppm yr<sup>-1</sup> respectively. It seems that the longer the moving window is, the larger difference is the long term growth rate to the measurements. For further investigating the reason, the annual mean carbon budgets on 11 Transcom regions are shown in Fig. 4. It can be found that the longer the moving window is, the larger are the carbon budget adjustments. Long windows result in underestimation of the corresponding long term growth rate.

To further investigate the long time and long distance impact of atmospheric transport on CO<sub>2</sub> observations, components of CO<sub>2</sub> concentration at observation sites

associated with different Transcom regions in each day before their observation times

are calculated in the following way. For a given region and some day before the

observation time, prior fluxes on other regions and in other days are all masked. Then

the atmospheric transport model can be run with a homogeneous initial atmospheric

CO<sub>2</sub> concentration and forced by the masked fluxes to obtain the corresponding CO<sub>2</sub>

concentration components.

These components at individual sites are then averaged in time to investigate general impacts of carbon fluxes from different sources. The results at 7 selected sites are shown in Fig. 5. For these sites, CO<sub>2</sub> concentrations resulting from carbon fluxes within 25 days are mainly from local carbon fluxes within 7 days (although mostly within 3 days). Carbon fluxes beyond 7 days or regions far from the observation locations have very small impacts, indicating that they have little information in observations (i.e. the contribution is less than observation error), even if the atmospheric transport model is accurate. Actually majority of observations (approximately 49) over continental sites used in this study have similar properties to these 7 sites. If the errors of the transport and ecosystem models are considered, the information of fluxes one week before may be even more difficult to estimate.

The setting of length of the assimilation window is closely related to spatial and temporal localizations of forecast errors. For the observation network and the atmospheric transport model used in this study, the one-week assimilation window seems most suitable.

3.3 Experimental design

In this section, the effectiveness of data assimilation methods introduced in Section 3

25 is examined with simulation experiments.

No ecosystem model is perfect. Therefore it is desirable to introduce ecosystem model error. In order to mimic this model error, we set the "true" carbon fluxes to be 80 percent of the BEPS simulated values plus 20 percent of the CarbonTracker assimilated values. The "true" gridded CO<sub>2</sub>-concentration is calculated starting from a CO<sub>2</sub>-concentration field taken from CarbonTracker document, and is forced by the "true" carbon fluxes. The synthetic observations are formed by adding noise to the interpolated "true" CO<sub>2</sub>-concentrations at the observation locations and times. All the observation errors are assumed to be statistically independent and normally distributed with standard deviation 0.2 ppmv. The experiments are carried out for 2002 with BEPS and MOZART. The ensemble size is 150 unless otherwise noted.

### 3.4 Inflation on observation error variance

In this section, we test the method of inflation on observation error covariance matrices described in Section 3.1. Three experiments with inflated forecast error are compared. In Experiment 1, the observation error variance is incorrectly specified (with variance of 0.5ppmv), and the inflation procedure is not carried out (refer to as Wrong R). In Experiment 2, the observation error variance is also specified as 0.5ppmv, but the inflation procedure is carried out (refer to as Wrong R + Inf). In Experiment 3, the observation error variance is correctly specified as 0.2 ppmv (refer to as True R). The regional RMSEs of the assimilated carbon fluxes and the monthly RMSEs of atmospheric concentrations at the observation sites in these three experiments are shown in Fig. 3 and 4 respectively.

 Figure 3 shows that the RMSEs of the estimated carbon fluxes (Eq. (8)) in all experiments are reduced on all 11 regions compared with the RMSEs of the prior

earbon fluxes. Similarly, Fig. 4 shows that the RMSEs of the estimated in situ atmospheric CO<sub>2</sub> concentrations (Eq. (10)) in all experiments are also reduced in all months compared with the RMSEs of the prior CO<sub>2</sub> concentrations. These facts indicate that the data assimilation schemes studied in this paper are useful. Moreover, the RMSEs from Experiment 3 (True R) is smaller than that from Experiment 1 (Wrong R). This suggests that correct specification of the observation error variances is important in improving the assimilation results.

The mean value of the estimated observation error variances in Experiment 2

(Wrong R + Inf) is 0.262ppmv. Although it is larger than the true value 0.2ppmv, but is much smaller than the incorrectly specified value 0.5ppmv. Nevertheless, the RMSEs from Experiment 2 (Wrong R + Inf) and Experiment 3 (True R) are comparable (see Fig. 3 and 4).

3.5 Constructing forecast error statistics using the analysis states

In this section, we test the methodology of using the analysis state to construct forecast error statistics described in Section 3.2. The corresponding Experiment 4 is referred to as "Wrong R + Inf + Anl".

Figure 3 shows that the RMSEs of the carbon fluxes assimilated in Experiment 4(Wrong R + Inf + Anl) are the smallest for all regions and in all experiments. Similarly, Fig. 4 shows that the RMSEs of the in situ atmospheric CO2 concentrations assimilated in Experiment 4 are the smallest for all months except September. These results indicate that the methodology of using the analysis state to construct forecast error statistics described in Section 3.2 can improve the assimilation results. The mean value of the estimated observation error variances in Experiment 3 (Wrong R + Inf +

1 Anl) is 0.268ppmv, which is virtually identical to that in Experiment 2 (Wrong R + Inf).

3.6 Validation

For investing the sensitivity of the inflation factors toward the choice of ensemble size, the time series of inflation factors are calculated with the ensemble size 200, and are plotted against the estimated inflation factors with the the ensemble size 150 (not shown here). In fact they are very close, suggesting that the ensemble size 150 used in both CarbonTracker and this study is reasonable.

The analysis spread and RMSE are also calculated for each region using Eq. (9)

and they are very close (not shown here). This indicates that the member of analysis states may have the same distribution as the true states.

By including CO<sub>2</sub>-concentration in the state vectors, the initial value of gridded CO<sub>2</sub>-concentration at every week is the analysis states of CO<sub>2</sub>-concentration at previous week. However, when excluding CO<sub>2</sub>-concentration from the state vectors, the initial value of gridded CO<sub>2</sub>-concentration can also be estimated by using atmospheric transport model forced by the assimilated surface carbon fluxes at previous week. Sensitivity experiments were carried out to compare these two approaches. The RMSEs of analysis in the experiment without including CO<sub>2</sub>-concentration in state vectors are close to those in Wrong R + Inf + Anl, which suggests that including CO<sub>2</sub>-concentration in state vectors may not significantly improves the assimilation results. However, in Wrong R + Inf + Anl the initial states of gridded atmospheric CO<sub>2</sub>-concentration need not be re-estimated, thus the computational cost of atmospheric transport model is about half of that in experiment without including CO<sub>2</sub>-concentration.

# 

### 45\_Application and results

In this section we use the data assimilation methods described in Section 3 to estimate the land surface carbon fluxes from 2002 to 2008. The fossil fuel, forest fire and ocean surface carbon flux forcing fields of the atmospheric transport model MOZART are all taken from CarbonTracker website. The initial atmospheric  $CO_2$ -concentration field is also from CarbonTracker products. The prior land surface carbon fluxes are simulated by the ecosystem model BEPS. In this study, only land surface carbon fluxes need to be adjusted. The partition of the adjustment factors (i.e.  $\lambda_r$  in Section 3) is based on 11 TransCom regions (Gurney et al., 2004) and 19 Olson ecosystem types, as in CarbonTracker. Prior observation error covariance matrix is adopted from CarbonTracker. We refer to this data assimilation scheme as Global Carbon Assimilation System using Ensemble Kalman filter (GCAS EK).

### 4.15.1 Adjustment to total carbon budget of BEPS

We first carry out a control run starting from Jan<u>uary</u> 1, 2002 with no adjustment of prior fluxes. The simulated CO<sub>2</sub> concentrations are interpolated at measurement observation times and locations, and compared with real observations in the year 2005. The result is shown in Fig. 5a6a). It shows that the simulated concentrations have a bias of 2.945\_ppmv and an RMSE of 4.525\_ppmv, which implies implying an underestimation of carbon sinks by BEPS. WithUsing GCAS-EK to estimate the ecosystem fluxes estimated by GCAS-EK, we carry out another control run and comparisons. The bias and RMSE are reduced to 0.967\_ppmv and 3.675\_ppmv,

respectively (Fig. 5b6b).

We have It is worthwhile to point out that the underestimation of carbon sinks by BEPS is conditioned on the estimated carbon fluxes released by fossil fuel and fire, even if the ocean fluxes used in our assimilation system are accurate. As described in Section 2, the observed variability of CO<sub>2</sub> concentration is due to the variability of carbon fluxes from all sources, including fossil fuel combustion, vegetation fire, oceanic uptake and biosphere exchange. If non-biospheric carbon sources not from biosphere are underestimated, the carbon sinks from the biosphere simulated by BEPS would also be underestimated. Nevertheless, our adjustment to carbon sinks simulated by BEPS appears reasonable.

4.25.2 Multiyear average of the global carbon flux distribution

2008 is shown in Fig. 6. Twhere the two spatial patterns of carbon fluxes related to BEPS (BEPS and GCAS-EKFig. 6a and 6b) are similar, although. However, they are quite different from that of CarbonTracker products-2011(Fig. 6e).

In the North American region, CarbonTracker exhibits a nearly west east strip of the carbon sink (Fig. 6c), while the carbon sinks assimilated or simulated by BEPS are mainly distributed in the east of 95° W (Fig. 6a and 6b). In the central Africa near the southern edge of Sahara desert, CarbonTracker simulates a strong carbon sink (Fig. 6c), but BEPS simulates a weak sink (Fig. 6a), while the assimilated result shows a weak source (Fig. 6b). In Indonesia, CarbonTracker simulates a moderate carbon source (Fig. 6c), while carbon sinks are simulated and assimilated by BEPS (Fig. 6a and 6b). In Australian Northern Territory, CarbonTracker simulates a carbon sink (Fig. 6a).

Figure 7 shows Tthe distribution of the average global carbon budget from 2002 to

1 6c), while the other two produce carbon sources (Fig. 6a and 6b). In North American
2 Temperate and Eurasia Boreal, the assimilated carbon sink is clearly larger than that
3 simulated.

Carbon budgets are calculated based on the BEPS ecosystem types and the 11 TransCom-Transcom regions (Fig. 78). Similar to the global distribution maps (Fig. 67), the assimilated BEPSGCAS-EK carbon budgets (Fig. 78) have almost the same property in sources or sinks with that simulated by BEPS. However, they are quite differenct from that of CarbonTracker 2011 in many aspects. For example, for the C4 and the shrub in Australia, BEPS simulates carbon sources while CarbonTracker 2011 shows carbon sinks. Moreover in North America, there is a large carbon sink increase of the assimilated GCAS-EK over the BEPS simulated. A Ffurther diagnostic (not shown here) reveals that, between October and April, the carbon sinks estimated by CarbonTracker 2011 are much larger than that estimated by GCAS-EK. But between May and September, the carbon sinks estimated by CarbonTracker 2011 and GCAS-EK are very close.

4.35.3 Interannual and seasonal variations

The interannual variations of the global total carbon budgets are shown in Fig. 89. It shows that CarbonTracker\_2011 predicts the largest multiyear average carbon sink (-3.89 PgC yearyr<sup>-1</sup>), compared with the smallest one simulated by BEPS (-2.23 PgC yearyr<sup>-1</sup>). The assimilated mean carbon sink (-3.87 PgC yearyr<sup>-1</sup>) is virtually identical to that estimated by CarbonTracker\_2011. The carbon sinks simulated by BEPS and predicted by CarbonTracker\_2011 obviously have more interannual oscillation than that assimilated by GCAS-EK.

The monthly <u>changes variations</u> of the multiyear-averaged carbon budgets before and after the assimilation of BEPS results are compared with that by CarbonTracker <u>2011</u> in Fig. <u>910</u>. Clearly, the seasonal variability of the carbon budgets by CarbonTracker <u>2011</u> is the largest. The assimilated fluxes based on BEPS have larger sinks in the summer and smaller sources in the winter than those before the assimilation.

#### 5.4 Comparison to other flux estimations

Two independent gridded carbon flux estimates are compared with GCAS-EK estimates.

The first independent dataset is net carbon exchange of U.S. terrestrial ecosystems by Xiao et al. (2011) which is generated by integrating eddy covariance flux measurements and satellite observations from Moderate Resolution Imaging Spectroradiometer (MODIS). The original dataset is during 2002 to 2006 with spatial resolution of 1km and temporal resolution of 8 day. For comparison, Xiao's data were grouped from 1km to 1° spatial resolution. The carbon flux distributions of the multiyear average from 2002 to 2006 over United States are shown in Fig. 11 for Xiao's data, GCAS-EK and CarbonTracker 2011. It shows that spatial pattern of the flux assimilated by GCAS-EK is closer to Xiao's data (with spatial standard deviation 153 gC m<sup>2</sup> yr<sup>-1</sup> and spatial correlation 0.47) than that by CarbonTracker 2011 (with spatial standard deviation 197 gC m<sup>2</sup> yr<sup>-1</sup> and spatial correlation 0.22).

The carbon budgets estimated by GCAS-EK were also compared to those by Lauvaux et al. (2012), Penn State University (PSU) inversion and Colorado State University (CSU) inversion (Schuh et al., 2013) for the Mid Continent Intensive (MCI)

area from June – December 2007. The spatial patterns by GCAS-EK and
CarbonTracker 2011 are similar to those estimated by PSU, CSU (Schuh et al., 2013)
and Lauvaux et al. (2012) (not shown here). The regional averaged carbon sinks
estimated by GCAS-EK and by CarbonTracker 2011 are 0.19 PgC and 0.26 PgC
respectively while the averaged carbon sinks estimated by PSU and CSU (Schuh et al.,
2013) and by Lauvaux et al. (2012) are between 0.14 PgC and 0.18 PgC, which are
closer to that estimated by GCAS-EK than that by CarbonTracker 2011.

Since the true values of carbon flux are unknown, the closeness to the

Since the true values of carbon flux are unknown, the closeness to the independent gridded carbon flux estimates does not mean a better assimilation. However, these two examples indicate that the carbon fluxes estimated by GCAS-EK may provide some useful new information of global carbon flux estimation to the atmospheric inversion community. Therefore, the development of the new assimilation system is worthwhile.

### 5 Discussion

### 5.1 Comparison with Carbon Tracker

Including CO<sub>2</sub> concentration in the state vector implies that an atmospheric transport model is part of the forecast operator, not part of the observation operator (such as in CarbonTracker). In this framework, the forecast operator comprises an atmospheric transport model and forecast of adjusted factors (Eq.(1)(2)). The observation operator is the linear operator which interpolates gridded atmospheric CO<sub>2</sub> concentration onto the observation points. Moreover for remotely sensed CO<sub>2</sub> cylinder concentration data, the observation operator can be chosen as a weighted average of gridded atmosphere

CO<sub>2</sub> concentrations.

Since atmospheric CO<sub>2</sub> concentration is not model variable in CarbonTracker, the observation operator in this study is different from that in CarbonTracker. In CarbonTracker, the observation operator is atmospheric transport model coupled with a linear spatial interpolation operator which maps surface CO<sub>2</sub> fluxes to atmospheric CO<sub>2</sub> concentration observation network. Then its observation error comprises the following three components: 1) measurement error covariance; 2) representation error covariance; and 3) model transport error covariance. In this study, the observation operator is only the linear spatial interpolation operator. So the observation error in our experiment only comprises components 1) and 2).

The mean value of the estimated  $\mu_i$  for inflating the prior observation error variances is 0.74. This indicates that the estimated observation error variances are smaller than that used in CarbonTracker. This may be due to that model transport errors are not included in our observation errors, but are included in the observation errors for CarbonTracker.

### 5.2 Forecast of adjusted factors

From the extensive experiments conducted in this study, we find that the spatial pattern of assimilated fluxes is highly correlated with the spatial pattern of prior fluxes. This is due to the fact that the unconditional expectation of the analysis  $E\left[\lambda_{i,i}^a\right]$  is 1, which could be attributed to the setting of forecast of adjusted factors (Eq. (1)). Then the probability of shifting between carbon sources and sinks is small. It means that GCAS EK generally trusts the spatial pattern simulated by the ecosystem model.

To avoid this problem, more flexible adjustment of  $\mathbf{f}_t$  with more adjusted factors

may be considered. However, the increased number of the adjusted factors results in increased degrees of freedom of adjustment model. To fit such kind of model more abundance of observations may be required. For surface flask observations with a total number of about 100 every week over the entire globe, the number of adjusted factors has to be carefully controlled. Therefore, under the current density of ground based observation network, improving the accuracy of the ecosystem model producing the prior fluxes may be more feasible strategy to improve the surface flux estimation.

### 5.3 Length of the assimilation time window

Different lengths of the assimilation time window are used in various systems (5 weeks in CarbonTracker, 3 and 7 days in Miyazaki et al. (2011) and 6 hours in Kang et al. (2012)). We choose one week as the length in our methodology for the following two reasons. Firstly, since most surface stations only have weekly observations, we need at least one week data to cover the globe. Secondly, beyond one week the model errors of MOZART and BEPS may be significant, but they are very difficult to quantify.

#### 6 Conclusion

We propose a methodology to assimilate atmospheric CO<sub>2</sub> concentration into surface carbon fluxes simulated by an ecosystem model. In our framework, CO<sub>2</sub> concentration is included in the state vector, and the assimilation window is restricted to one week.

Bboth forecast and observation errors are inflated, and forecast error statistics are

estimated in an adaptive procedure using the analysis states. Generally speaking, these

adaptive estimations improve the accuracy of assimilated error statistics in EnKF,

3 which leads to further improvement in the accuracy of analysis states. Importantly,

pre-assigned values of the observation error variance are improved if these adaptive

procedures are applied.

Four simulation experiments were carried out to show the effectiveness of the proposed methodology. In the first two experiments, we assumed the observation error variances were incorrectly specified and compared assimilation results with and without using inflations on the observation error statistics. The third experiment, in which the observation error variances were supposed to be known, served as a benchmark of how the observation error variances were estimated using our methodology. The fourth experiment showed the effectiveness of using analysis states to further improve the estimation of forecast error. The results from all experiments met our expectation and increased our confidence in applying the improved EnKF to assimilate real observations. The application of the methodology to real data shows that the assimilated total carbon fluxesbudgets by GCAS-EK are comparable to those reported by CarbonTracker 2011. However, there are significant regional differences between carbon flux distributions assimilated by GCAS-EK and CarbonTracker 2011, which may be attributed to the differences between the ecosystem models, atmospheric transport models and or the assimilation methodologies.

In our future study, we will investigate the sensitivity of assimilation results to the accuracy of <u>eeologicalecosystem\_models\_models\_models\_models\_models.</u> Also, more observation datasets, such as remote sensing <u>CO<sub>2</sub> column\_models</u>, will be introduced into the GCAS-EK.

1

2

- 3 Acknowledgements This work was supported by National Program on Key Basic
- 4 Research Project of China (Grant No. 2010CB950703), R&D Special Fund for
- 5 Nonprofit Industry (Meteorology, Grant No. GYHY201206008), Key Technologies
- 6 Research and Development Program of China (Grant No. 2013BAC05B04) and the
- 7 Natural Sciences and Engineering Research Council of Canada (NSERC). We would
- 8 <u>like to thank Prof Peter Rayner and an anonymous reviewer for their valuable</u>
- 9 comments which lead to much improvement of this paper. We acknowledge all
- 10 <u>atmospheric data providers to</u>
- obspack co2 1 CARBONTRACKER CT2013 2014-05-08, and those who
- 12 <u>contributed their data to WDCGG. We grateful acknowledge CarbonTracker 2011</u>
- results provided by NOAA ESRL, Boulder, Colorado, USA, on the website
- 14 http://carbontracker.noaa.gov.

15

16

#### References

- Boden, T. A., Marland, G., and Andres, R. J.: Global, Regional, and National Fossil-Fuel
- 18 CO2 Emissions, Carbon Dioxide Information Analysis Center, Oak Ridge National
- 19 Laboratory, U.S. Department of Energy, Oak Ridge, Tenn., U.S.A.,
- 20 10.3334/CDIAC/00001\_V2011, 2011.
- 21 Burgers, G., Jan van Leeuwen, P., and Evensen, G.: Analysis Scheme in the Ensemble
- 22 Kalman Filter, Mon. Weather Rev., 126, 1719-1724,
- 23 10.1175/1520-0493(1998)126<1719:asitek>2.0.co;2, 1998.
- 24 Chen, J. M., Liu, J., Cihlar, J., and Goulden, M. L.: Daily canopy photosynthesis model
- through temporal and spatial scaling for remote sensing applications, Ecol. Model.,
- 26 124, 99--119, 10.1016/S0304-3800(99)00156-8, 1999.
- 27 Desroziers, G., Berre, L., Chapnik, B., and Poli, P.: Diagnosis of observation,
- 28 background and analysis-error statistics in observation space, Q. J. R. Meteorolog.
- 29 Soc., 131, 3385--3396, 2005.
- 30 Emmons, L. K., Walters, S., Hess, P. G., Lamarque, J. F., Pfister, G. G., Fillmore, D.,

- 1 Granier, C., Guenther, A., Kinnison, D., Laepple, T., Orlando, J., Tie, X., Tyndall, G.,
- 2 Wiedinmyer, C., Baughcum, S. L., and Kloster, S.: Description and evaluation of the
- 3 Model for Ozone and Related chemical Tracers, version 4 (MOZART-4), Geosci. Model
- 4 Dev., 3, 43-67, 10.5194/gmd-3-43-2010, 2010.
- 5 Enting, I. G.: Inverse Problems in Atmospheric Constituent Transport, Cambridge
- 6 University Press, New York, 2002.
- 7 Gurney, K. R., Law, R. M., Denning, A. S., Rayner, P. J., Pak, B. C., Baker, D., Bousquet,
- 8 P., Bruhwiler, L., Chen, Y. H., Ciais, P., Fung, I. Y., Heimann, M., John, J., Maki, T.,
- 9 Maksyutov, S., Peylin, P., Prather, M., and Taguchi, S.: Transcom 3 inversion
- 10 intercomparison: Model mean results for the estimation of seasonal carbon sources
- and sinks, Global Biogeochem. Cycles, 18, GB1010-GB1010, 10.1029/2003GB002111,
- 12 2004.
- 13 Ide, K., Courtier, P., Ghil, M., and Lorenc, A. C.: Unified notation for data assimilation:
- Operational, sequential and variational, J. Meteorol. Soc. Jpn., 75, 181-189, 1997.
- 15 Jacobson, A. R., Mikaloff Fletcher, S. E., Gruber, N., Sarmiento, J. L., and Gloor, M.: A
- 16 joint atmosphere-ocean inversion for surface fluxes of carbon dioxide: 1. Methods
- 17 and global-scale fluxes, Global Biogeochem. Cycles, 21, GB1019
- 18 10.1029/2005GB002556, 2007.
- 19 Ju, W. M., Chen, J. M., Black, T. A., Barr, A. G., Liu, J., and Chen, B. Z.: Modelling
- 20 multi-year coupled carbon and water fluxes in a boreal aspen forest, Agric. For.
- 21 Meteorol., 140, 136--151, 10.1016/j.agrformet.2006.08.008, 2006.
- 22 Kalnay, E., Kanamitsu, M., Kistler, R., Collins, W., Deaven, D., Gandin, L., Iredell, M.,
- 23 Saha, S., White, G., Woollen, J., Zhu, Y., Leetmaa, A., Reynolds, R., Chelliah, M.,
- Ebisuzaki, W., Higgins, W., Janowiak, J., Mo, K. C., Ropelewski, C., Wang, J., Jenne, R.,
- and Joseph, D.: The NCEP/NCAR 40-Year Reanalysis Project, Bulletin Am. Meteorol.
- 26 Soc., 77, 437-471, 10.1175/1520-0477(1996)077<0437:TNYRP>2.0.CO;2, 1996.
- 27 Kang, J. S., Kalnay, E., Liu, J., Fung, I., Miyoshi, T., and Ide, K.: "Variable localization" in
- an ensemble Kalman filter: Application to the carbon cycle data assimilation, J.
- 29 Geophys. Res., 116, D09110, 2011.
- 30 Kang, J. S., Kalnay, E., Miyoshi, T., Liu, J., and Fung, I.: Estimation of surface carbon
- 31 fluxes with an advanced data assimilation methodology, J. Geophys. Res.: Atmos.
- 32 (1984--2012), 117, 2012.
- 33 Kistler, R., Collins, W., Saha, S., White, G., Woollen, J., Kalnay, E., Chelliah, M.,
- Ebisuzaki, W., Kanamitsu, M., Kousky, V., van den Dool, H., Jenne, R., and Fiorino, M.:
- 35 The NCEP-NCAR 50-Year Reanalysis: Monthly Means CD-ROM and Documentation,
- 36 Bulletin Am. Meteorol. Soc., 82, 247-267,
- 37 10.1175/1520-0477(2001)082<0247:TNNYRM>2.3.CO;2, 2001.
- 38 Lauvaux, T., Schuh, A. E., Uliasz, M., Richardson, S., Miles, N., Andrews, A. E., Sweeney,
- 39 C., Diaz, L. I., Martins, D., Shepson, P. B., and Davis, K. J.: Constraining the CO2 budget

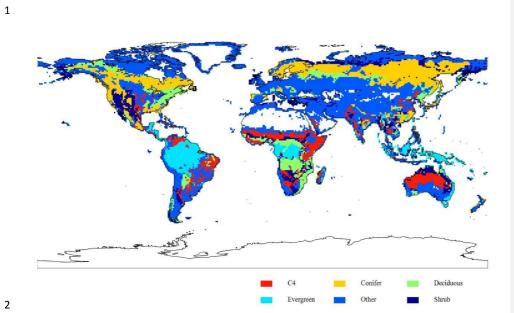
- of the corn belt: exploring uncertainties from the assumptions in a mesoscale inverse
- 2 system, Atmos. Chem. Phys., 12, 337-354, 10.5194/acp-12-337-2012, 2012.
- 3 Liang, X., Zheng, X., Zhang, S., Wu, G., Dai, Y., and Li, Y.: Maximum likelihood
- 4 estimation of inflation factors on error covariance matrices for ensemble Kalman
- 5 filter assimilation, Q. J. R. Meteorolog. Soc., 138, 263--273, 10.1002/qj.912, 2012.
- 6 Liu, J., Chen, J. M., Cihlar, J., and Chen, W.: Net primary productivity distribution in
- 7 the BOREAS region from a process model using satellite and surface data, J. Geophys.
- 8 Res. [Atmos.], 104, 27735--27754, 10.1029/1999JD900768, 1999.
- 9 Liu, J., Fung, I., Kalnay, E., Kang, J.-S., Olsen, E. T., and Chen, L.: Simultaneous
- 10 assimilation of AIRS Xco2 and meteorological observations in a carbon climate model
- 11 with an ensemble Kalman filter, J. Geophys. Res. [Atmos.], 117, D05309,
- 12 10.1029/2011JD016642, 2012.
- 13 Masarie, K. A., Peters, W., Jacobson, A. R., and Tans, P. P.: ObsPack: a framework for
- 14 the preparation, delivery, and attribution of atmospheric greenhouse gas
- measurements, Earth Syst. Sci. Data, 6, 375-384, 10.5194/essd-6-375-2014, 2014.
- 16 Michalak, A. M., Hirsch, A., Bruhwiler, L., Gurney, K. R., Peters, W., and Tans, P. P.:
- 17 Maximum likelihood estimation of covariance parameters for Bayesian atmospheric
- 18 trace gas surface flux inversions, J. Geophys. Res. [Atmos.], 110, D24107,
- 19 10.1029/2005JD005970, 2005.
- 20 Miyazaki, K., Maki, T., Patra, P., and Nakazawa, T.: Assessing the impact of satellite,
- 21 aircraft, and surface observations on CO2 flux estimation using an ensemble-based
- 22 4-D data assimilation system, J. Geophys. Res. [Atmos.], 116, D16306,
- 23 10.1029/2010JD015366, 2011.
- 24 Mo, X. G., Chen, J. M., Ju, W. M., and Black, T. A.: Optimization of ecosystem model
- 25 parameters through assimilating eddy covariance flux data with an ensemble Kalman
- 26 filter, Ecol. Model., 217, 157--173, 10.1016/j.ecolmodel.2008.06.021, 2008.
- 27 Oda, T., and Maksyutov, S.: A very high-resolution (1 km×1 km) global fossil fuel CO2
- 28 emission inventory derived using a point source database and satellite observations
- 29 of nighttime lights, Atmos. Chem. Phys., 11, 543-556, 10.5194/acp-11-543-2011,
- 30 2011.
- Peters, W., Miller, J. B., Whitaker, J., Denning, A. S., Hirsch, A., Krol, M. C., Zupanski, D.,
- 32 Bruhwiler, L., and Tans, P. P.: An ensemble data assimilation system to estimate CO2
- 33 surface fluxes from atmospheric trace gas observations, J. Geophys. Res. [Atmos.],
- 34 110, D24304-D24304, 10.1029/2005JD006157, 2005.
- Peters, W., Jacobson, A. R., Sweeney, C., Andrews, A. E., Conway, T. J., Masarie, K.,
- Miller, J. B., Bruhwiler, L. M., Petron, G., Hirsch, A. I., Worthy, D. E., van der Werf, G. R.,
- 37 Randerson, J. T., Wennberg, P. O., Krol, M. C., and Tans, P. P.: An atmospheric
- 38 perspective on North American carbon dioxide exchange: CarbonTracker, Proceedings
- 39 of the National Academy of Sciences of the United States of America, 104,

- 1 18925-18930, 10.1073/pnas.0708986104, 2007.
- 2 Potter, C. S., Randerson, J. T., Field, C. B., Matson, P. A., Vitousek, P. M., Mooney, H. A.,
- and Klooster, S. A.: Terrestrial ecosystem production: A process model based on
- 4 global satellite and surface data, Global Biogeochem. Cycles, 7, 811-841,
- 5 10.1029/93GB02725, 1993.
- 6 Schuh, A. E., Lauvaux, T., West, T. O., Denning, A. S., Davis, K. J., Miles, N., Richardson,
- 7 S., Uliasz, M., Lokupitiya, E., Cooley, D., Andrews, A., and Ogle, S.: Evaluating
- 8 atmospheric CO2 inversions at multiple scales over a highly inventoried agricultural
- 9 landscape, Global Change Biol., 19, 1424-1439, 10.1111/gcb.12141, 2013.
- Takahashi, T., Sutherland, S. C., Wanninkhof, R., Sweeney, C., Feely, R. A., Chipman, D.
- 11 W., Hales, B., Friederich, G., Chavez, F., Sabine, C., and others: Climatological mean
- and decadal change in surface ocean pCO< sub> 2</sub>, and net sea--air CO< sub>
- 13 2</sub> flux over the global oceans, Deep Sea Res. Part II: Topical Studies in
- 14 Oceanography, 56, 554--577, 2009.
- 15 Tarantola, A.: Inverse Problem Theory and Methods for Model Parameter Estimation,
- 16 Other Titles in Applied Mathematics, Society for Industrial and Applied Mathematics,
- 17 348 pp., 2005.
- van der Werf, G. R., Randerson, J. T., Giglio, L., Collatz, G. J., Kasibhatla, P. S., and
- 19 Arellano Jr, A. F.: Interannual variability in global biomass burning emissions from
- 20 1997 to 2004, Atmos. Chem. Phys., 6, 3423-3441, 10.5194/acp-6-3423-2006, 2006.
- 21 Wu, G. C., Zheng, X. G., Wang, L. Q., Zhang, S. P., Liang, X., and Li, Y.: A new structure
- 22 for error covariance matrices and their adaptive estimation in EnKF assimilation, Q. J.
- 23 R. Meteorolog. Soc., 139, 795-804, Doi 10.1002/Qj.2000, 2013.
- 24 Xiao, J., Zhuang, Q., Law, B. E., Baldocchi, D. D., Chen, J., Richardson, A. D., Melillo, J.
- 25 M., Davis, K. J., Hollinger, D. Y., Wharton, S., Oren, R., Noormets, A., Fischer, M. L.,
- Verma, S. B., Cook, D. R., Sun, G., McNulty, S., Wofsy, S. C., Bolstad, P. V., Burns, S. P.,
- 27 Curtis, P. S., Drake, B. G., Falk, M., Foster, D. R., Gu, L., Hadley, J. L., Katul, G. G., Litvak,
- 28 M., Ma, S., Martin, T. A., Matamala, R., Meyers, T. P., Monson, R. K., Munger, J. W.,
- Oechel, W. C., Paw, U. K. T., Schmid, H. P., Scott, R. L., Starr, G., Suyker, A. E., and Torn,
- 30 M. S.: Assessing net ecosystem carbon exchange of U.S. terrestrial ecosystems by
- W. J.: Assessing her ecosystem carbon exchange of 0.5. terrestrial ecosystems by
- 31 integrating eddy covariance flux measurements and satellite observations, Agric. For.
- 32 Meteorol., 151, 60-69, 10.1016/j.agrformet.2010.09.002, 2011.
- 33 Zheng, X.: An Adaptive Estimation of Forecast Error Covariance Parameters for
- 34 Kalman Filtering Data Assimilation, Adv. Atmos. Sci., 26, 154--160,
- 35 10.1007/s00376-009-0154-5, 2009.
- 36 Zheng, X., Wu, G., Zhang, S., Liang, X., Dai, Y., and Li, Y.: Using analysis state to
- 37 construct a forecast error covariance matrix in ensemble Kalman filter assimilation,
- 38 Adv. Atmos. Sci., 30, 1303-1312, 10.1007/s00376-012-2133-5, 2013.

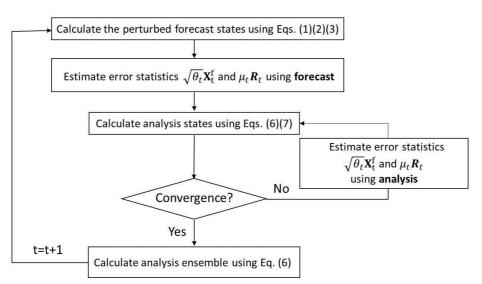
**Table 1.** 92 observation sites used in this study. "r" refers to prescribed observation error (umol umol<sup>-1</sup>).

error (umoi umoi ).									
Site Code	Lat (°)	Lon (°)	r	Lab	Site Code	Lat (°)	Lon (°)	r	Lab
ABP_01D0	-12.27	-38.17	2.50	NOAA*	MID_01D0	28.21	-177.38	1.50	NOAA
ABP_26D0	-12.27	-38.17	2.50	IPEN*	MKN_01D0	-0.05	37.30	2.50	NOAA
ALT_01D0	82.45	-62.51	1.50	NOAA	MLO_01C0_02LST	19.54	-155.58	0.75	NOAA
ALT 06C0 14LST	82.45	-62.51	2.50	EC*	MLO 01D0	19.54	-155.58	1.50	NOAA
AMT_01C3_14LST	45.03	-68.68	3.00	NOAA	MQA_02D0	-54.48	158.97	0.75	CSIRO
AMT_01P0	45.03	-68.68	3.00	NOAA	NMB_01D0	-23.58	15.03	2.50	NOAA
ASC_01D0	-7.97	-14.40	0.75	NOAA	NWR_01D0	40.05	-105.58	1.50	NOAA
ASK_01D0	23.18	5.42	1.50	NOAA	NWR_03C0_02LST	40.05	-105.58	3.00	NCAR*
AZR_01D0	38.77	-27.38	1.50	NOAA	OBN_01D0	55.11	36.60	7.50	NOAA
BAL_01D0	55.35	17.22	7.50	NOAA	OXK_01D0	50.03	11.80	2.50	NOAA
BAO_01C3_14LST	40.05	-105.00	3.00	NOAA	PAL_01D0	67.97	24.12	2.50	NOAA
BAO_01P0	40.05	-105.00	3.00	NOAA	POC_01D1	-0.39	-132.32	0.75	NOAA
BHD_01D0	-41.41	174.87	1.50	NOAA	PSA_01D0	-64.92	-64.00	0.75	NOAA
BKT_01D0	-0.20	100.32	7.50	NOAA	PTA_01D0	38.95	-123.74	7.50	NOAA
BME_01D0	32.37	-64.65	1.50	NOAA	RPB_01D0	13.17	-59.43	1.50	NOAA
BMW_01D0	32.27	-64.88	1.50	NOAA	SCT_01C3_14LST	33.41	-81.83	3.00	NOAA
BRW_01C0_14LST	71.32	-156.61	2.50	NOAA	SEY_01D0	-4.67	55.17	0.75	NOAA
BRW_01D0	71.32	-156.61	1.50	NOAA	SGP_01D0	36.80	-97.50	2.50	NOAA
BSC_01D0	44.17	28.68	7.50	NOAA	SGP_64C3_16LST	36.80	-97.50	3.00	LBNL*
CBA_01D0	55.21	-162.72	1.50	NOAA	SHM_01D0	52.72	174.10	2.50	NOAA
CDL_06C0_14LST	53.99	-105.12	3.00	EC	SIS_02D0	60.17	-1.17	2.50	CSIRO
CFA_02D0	-19.28	147.06	2.50	CSIRO*	SMO_01C0_14LST	-14.25	-170.56	0.75	NOAA
CGO_01D0	-40.68	144.69	0.75	NOAA	SMO_01D0	-14.25	-170.56	1.50	NOAA
CGO_02D0	-40.68	144.69	0.75	CSIRO	SNP_01C3_02LST	38.62	-78.35	3.00	NOAA
CHR_01D0	1.70	-157.17	0.75	NOAA	SPL_03C0_02LST	40.45	-106.73	3.00	NCAR
CRZ_01D0	-46.45	51.85	0.75	NOAA	SPO_01C0_14LST	-89.98	-24.80	0.75	NOAA
CYA_02D0	-66.28	110.52	0.75	CSIRO	SPO_01D0	-89.98	-24.80	1.50	NOAA
EGB_06C0_14LST	44.23	-79.78	3.00	EC	STM_01D0	66.00	2.00	1.50	NOAA
EIC_01D0	-27.15	-109.45	7.50	NOAA	STR_01P0	37.76	-122.45	3.00	NOAA
ETL_06C0_14LST	54.35	-104.98	3.00	EC	SUM_01D0	72.58	-38.48	1.50	NOAA
FSD_06C0_14LST	49.88	-81.57	3.00	EC	SYO_01D0	-69.00	39.58	0.75	NOAA
GMI_01D0	13.43	144.78	1.50	NOAA	TAP_01D0	36.73	126.13	7.50	NOAA
HBA_01D0	-75.58	-26.50	0.75	NOAA	TDF_01D0	-54.87	-68.48	0.75	NOAA
HPB_01D0	47.80	11.01	7.50	NOAA	THD_01D0	41.05	-124.15	2.50	NOAA
HUN_01D0	46.95	16.65	7.50	NOAA	UTA_01D0	39.90	-113.72	2.50	NOAA
ICE_01D0	63.40	-20.29	1.50	NOAA	UUM_01D0	44.45	111.10	2.50	NOAA
KEY_01D0	25.67	-80.16	2.50	NOAA	WBI_01C3_14LST	41.72	-91.35	3.00	NOAA
KUM_01D0	19.52	-154.82	1.50	NOAA	WBI_01P0	41.72	-91.35	3.00	NOAA
KZD_01D0	44.06	76.82	2.50	NOAA	WGC_01C3_14LST	38.27	-121.49	3.00	NOAA
KZM_01D0	43.25	77.88	2.50	NOAA	WGC_01P0	38.27	-121.49	3.00	NOAA
LEF_01C3_14LST	45.95	-90.27	3.00	NOAA	WIS_01D0	31.13	34.88	2.50	NOAA
LEF_01P0	45.95	-90.27	3.00	NOAA	WKT_01C3_14LST	31.31	-97.33	3.00	NOAA
LLB_06C0_14LST	54.95	-112.45	3.00	EC	WKT_01P0	31.31	-97.33	3.00	NOAA
LMP_01D0	35.52	12.62	1.50	NOAA	WLG_01D0	36.29	100.90	1.50	NOAA
MAA_02D0	-67.62	62.87	0.75	CSIRO	WSA_06C0_14LST	49.93	-60.02	3.00	EC
MHD_01D0	53.33	-9.90	2.50	NOAA	ZEP_01D0	78.90	11.88	1.50	NOAA

\*"NOAA": NOAA Global Monitoring Division; "CSIRO": Commonwealth Scientific and Industrial Research Organization; "NCAR": National Center For Atmospheric Research; "EC": Environment Canada; "IPEN": Instituto de Pesquisas Energeticas e Nucleares; "LBNL": Lawrence Berkeley National Laboratory.



**Figure 1.** Global distribution of ecosystem types in Land areas of 6 plant function types used in ecosystem model BEPS.



**Figure 2.** Flowchart of <u>modified Ensemble Kalman filter</u>, the proposed adaptive procedure.

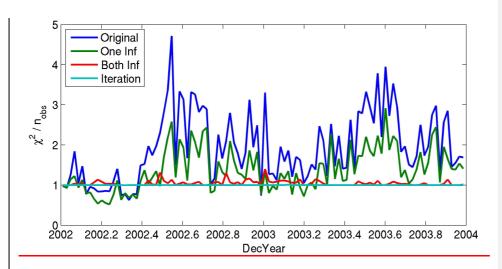
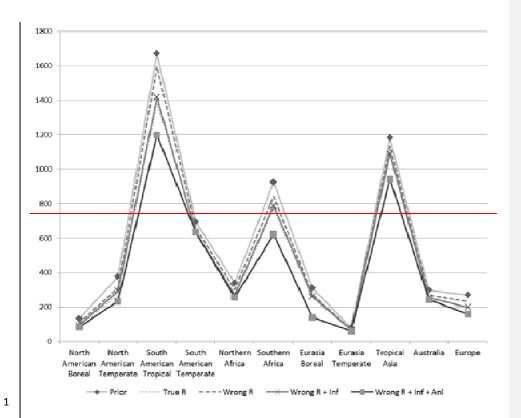


Figure 3.  $\chi^2$  statistics of the analysis state for four estimates of error covariance. "Original" refers to the case without inflations; "One Inf" refers to the case with inflation on forecast error covariance only; "Both Inf" refers to the case with inflations on both forecast and observation error covariances and "Iteration" refers to the case with both inflations and further using analysis to improve forecast error statistics. The closer  $\chi^2/n_{obs}$  is to 1, the better the corresponding error estimates.

域代码已更改



**Figure 3.** RMSEs (gC m<sup>2</sup>-year<sup>1</sup>) of carbon fluxes in four experiments: 1) the "standard" EnKF with incorrectly specified observation errors (Wrong R); 2) the "standard" EnKF with correctly specified observation errors (True R); 3) EnKF with inflation on both forecast and observation errors (Wrong R +Inf); 4) using analysis to further improve the estimation of forecast error statistics(Wrong R + Inf + Anl).

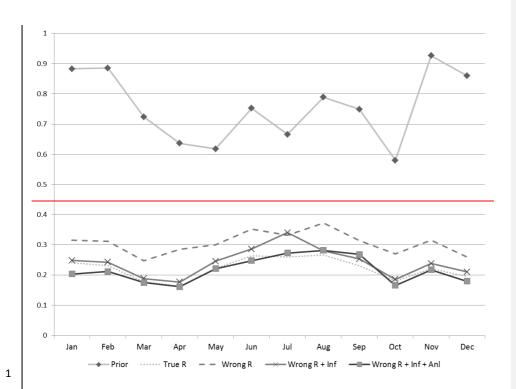


Figure 4. Posterior RMSEs (ppmv) of concentrations on observation sites in four experiments.—



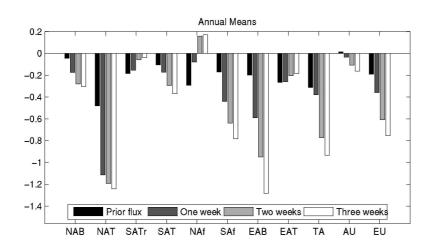


Figure 4. Annual means of carbon budgets (PgC yr<sup>-1</sup>) on 11 Transcom regions in four different cases. Four cases are associated with prior values modeled with ecosystem model BEPS, assimilated results using GCAS-EK with one-week assimilation windows, two-week windows and three-week windows. 11 regions in X-axis refer to 'North American Boreal' (NAB), 'North American Temperate' (NAT), 'South American Tropical' (SATr), 'South American Temperate' (SAT), 'Northern Africa' (NAf), 'Southern Africa' (SAf), 'Eurasia Boreal' (EAB), 'Eurasia Temperate' (EAT), 'Tropical Asia' (TA), 'Australia' (AU) and 'Europe' (EU), respectively

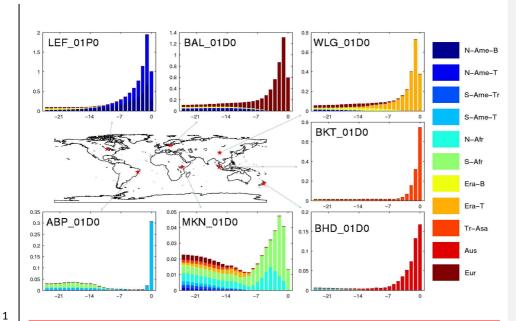
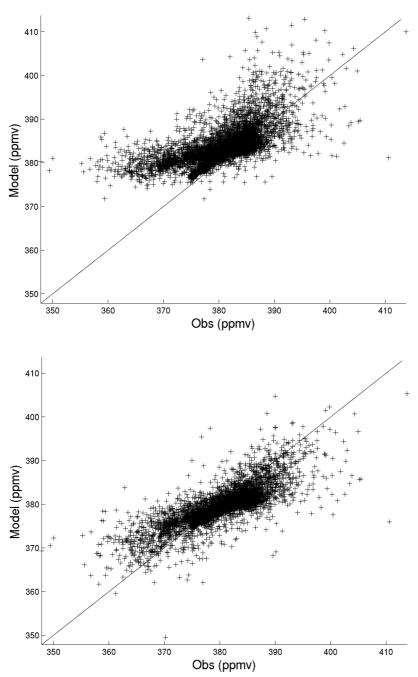
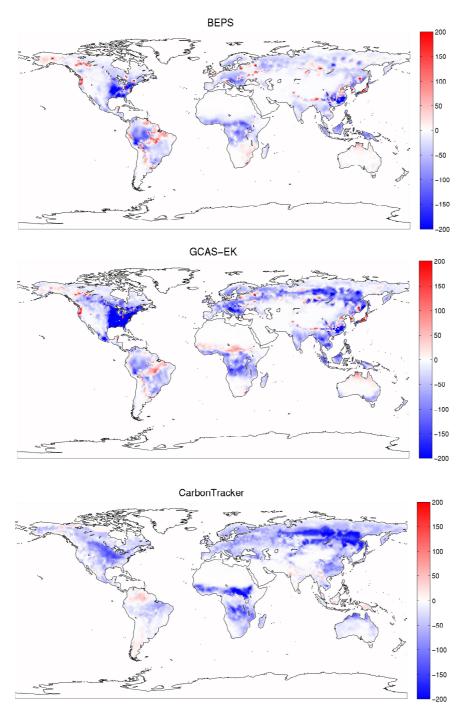


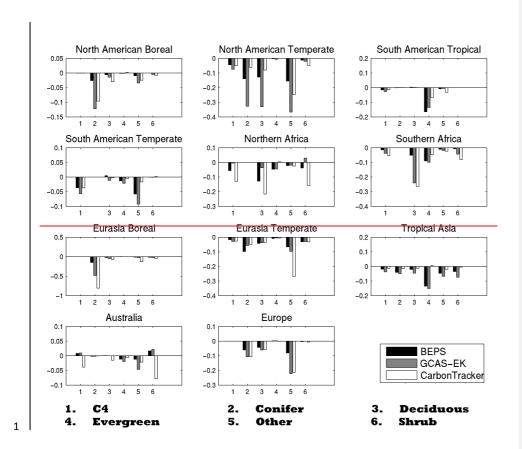
Figure 5. Mean components of CO<sub>2</sub> concentration at observation sites (Site IDs: LEF\_01P0, BAL\_01D0, WLG\_01D0, BKT\_01D0, BHD\_01D0, MKN\_01D0 and ABP\_01D0) from 11 Transcom regions in each of 25 days before the observation time. X-axis refers to days before the observation time. Y-axis refers to the amount of CO<sub>2</sub> concentration in ppm. Different colors within a bar refer to CO<sub>2</sub> concentration from 11 different Transcom regions. 11 regions refer to 'North American Boreal' (N-Ame-B), 'North American Temperate' (N-Ame-T), 'South American Tropical' (S-Ame-Tr), 'South American Temperate' (S-Ame-T), 'Northern Africa' (N-Afr), 'Southern Africa' (S-Afr), 'Eurasia Boreal' (Era-B), 'Eurasia Temperate' (Era-T), 'Tropical Asia' (Tr-Asa), 'Australia' (Aus) and 'Europe' (Eur) respectively.

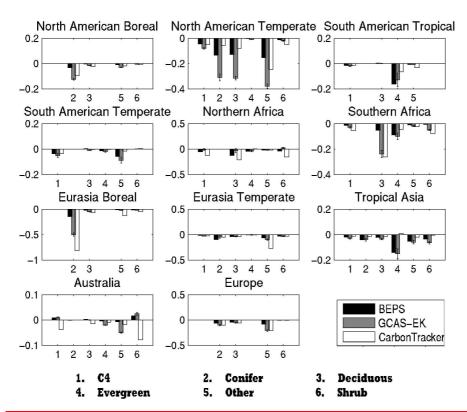


**Figure 6.** Comparisons between real observations and simulated concentrations by control runs: top) control run forcing by prior carbon fluxes; bottom) control run forcing by assimilated carbon fluxes by GCAS-EK. Both simulations start from Jan 1,2002 and all simulated concentrations at observation locations and times in 2005 are compared here.

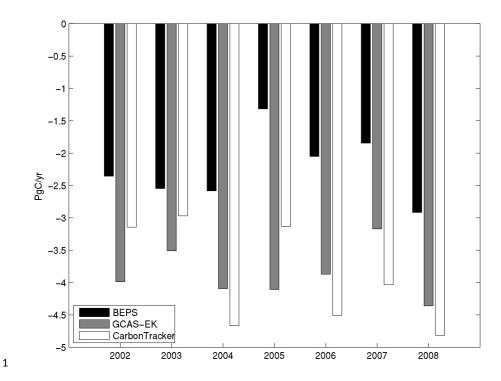


**Figure 7.** Global carbon budget (gC m<sup>-2</sup>) distributions on multiyear average from 2002 to 2008: prior carbon fluxes simulated by BEPS; assimilated carbon fluxes by GCAS-EK; CarbonTracker 2011 estimated carbon fluxes.

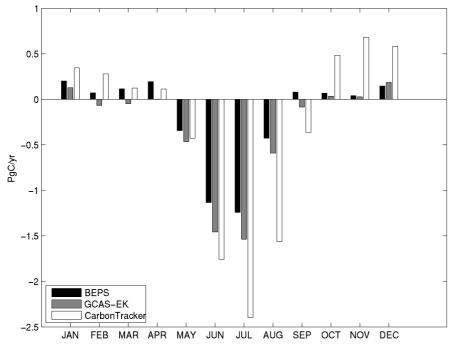




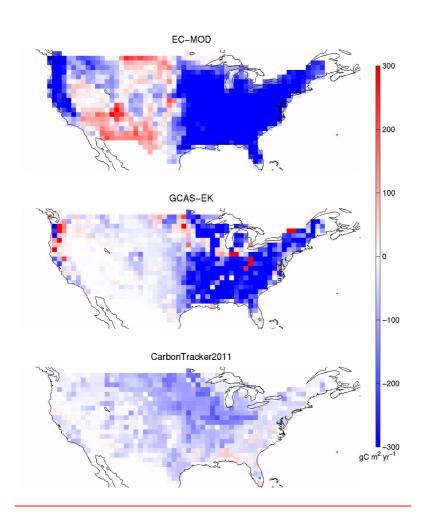
**Figure 78.** Average Annual mean carbon budgets (PgC yearyr<sup>-1</sup>) on areas of with 6 BEPS ecosystem plant function types inand TransCom regions from 2002 to 2008. The errors of GCAS-EK fluxes are the root mean square errors of the ensemble.



**Figure 89.** Comparison of the interannual change variations of global total carbon budgets from 2002 to 2008 by three products: BEPS, GCAS-EK and CarbonTracker 2011.



**Figure 910.** Comparison of multiyear average monthly change variations from 2002 to 2008 by three products: BEPS, GCAS-EK and CarbonTracker 2011.



**Figure 11.** The distribution of averaged net ecosystem exchange (gC m<sup>-2</sup> yr<sup>-1</sup>) from 2002 to 2006 for conterminous U.S. by EC-MOD, GCAS-EK and CarbonTracker 2011, respectively. The pattern correlation coefficient is 0.47 between EC-MOD and GCAS-EK, and 0.22 between CarbonTracker 2011 and EC-MOD.