**Ocean Science
Discussions**

Interactive comment on "Sea-air CO_2 flux estimated from SOCAT surface-ocean CO_2 partial pressure data and atmospheric CO_2 mixing ratio data" *by* C. Rödenbeck et al.

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Response to Referee comments by S. Mikaloff Fletcher

We thank Sara Mikaloff Fletcher for her comments which we found helpful in trying to make the manuscript more accessible to the readers. In the following reply, her original comments are included in italics.

This paper describes a new approach to incorporate observations of the difference between atmospheric and oceanic pCO2 into atmospheric inversions to estimate air- sea and air-land

fluxes of CO2. The authors develop a novel inverse approach that involves adjusting a simple model of carbon in the mixed layer using atmospheric and oceanic carbon data, which could potentially be quite valuable. To the best of my knowledge, this paper also represents the first attempt to incorporate the SOCAT data into atmospheric inversions, and this dataset is likely to add substantial new information about both ocean and land fluxes of CO2. However, I found it difficult to understand the details of the approach from the manuscript as written, and therefore I do not feel able to undertake a complete evaluation the inverse methodology at this time. I recommend that the authors substantially edit the manuscript to improve the clarity. If they choose to do so, I would look forward to reading the next version very much.

We substantially revised the explanation of the method and of the goals of the paper, and would appreciate her judgement whether we succeeded to improve clarity.

General Comments: I found the discussion of the description of the methodology difficult to fully understand, even though I have a background in atmospheric inversions. Each of the components of the model was well described in the appendices, but it was very hard for me to understand how all of these pieces fit together or develop a sense for how the ocean carbon data interact with the atmospheric inversion. The authors attempted to show this with a schematic (Figure 1), but I didn't find this figure helpful or informative. Again, it is very good for showing the pieces, but not for really understanding how they fit together. The authors could improve this by expanding section 2.1 to provide a better overview for the inverse framework and developing a better concept for how to present this framework in Figure 1.

We split Fig 1 in separate figures, one only summarizing the process representations (and all the involved quantities) in a forward sense, and a related one making the inverse information flow explicit. The new figure is referenced at various places where we think it can help understanding. The case of the pure atmospheric inversion is also given as a reference to readers familiar with it.

The authors made good use of appendices to include all of the detail a reader would need to replicate the work without making the manuscript too dense for a more casual reader. However, it would make the paper much more readable if a bit more detail appeared in the main text. To my mind, all material that most readers would need for a general understanding should appear in the main text, and extra details that most people won't need should go in the appendix. Some specific examples are described in the detailed comments section below.

We see the referee's point, and indeed had tried to put some of the equations into the main text during manuscript preparation. However, doing so would make it much harder to present a consistent line of thought in the Appendix. We did add some verbal statements as suggested.

This manuscript goes into great detail explaining the methods and the comparison with independent data, but I found the analysis of the results to be a bit thin. Section 4.1 indicates that the ocean pCO2 data provide a powerful constraint on the land regions, but the details of the differences between the land fluxes from this approach and traditional inversions and what they mean for the carbon cycle are never really discussed.

We agree that these issues are interesting, but had intended to present them in a subsequent paper in order not to overload the present one, given how long it is already. Though the effect on the land fluxes is a potential application of the presented product, we considered the ocean flux estimate itself the main target here.

Section 4.4 touches on the idea that the ocean internal carbon sources and sinks could tell us something fresh about ocean biogeochemistry, but never go into any depth. The authors might prefer to make such an analysis the basis of a follow-up paper in order to keep the manuscript length managable, but at least some of this analysis should be included.

The main purpose of this section was to substantiate that the employed model formu-

lation makes sense also in a process sense, not just as a mathematical device. We feel that any deeper analysis would indeed add too much material. We reformulated the section to make the intention more clear.

The manuscript includes a great deal of discussion of the pCO2 data, but the GLODAP DIC data are also included indirectly through the mixed layer depth model. It would be interesting to also discuss this and how the DIC data influence the inversion. There can also be biases induced by using a gridded dataset based on somewhat sparse data, and some discussion of this might be appropriate.

The choice of $C^{\text{DIC,LT}}$ actually only enters the result at 3 minor places: (i) in the freshwater flux, which is a crude parameterization anyway, and any errors of which are compensated by additional contributions to the internal flux but does not noticably change the pCO2 or sea-air fluxes; (ii) in the absolute value of C^{DIC} which is however not discussed in this paper; (iii) in a small contribution to the prior (to the extend that an inconsistency exists between $C^{\text{DIC,LT}}$ taken from the GLODAP gridded product and $p^{\text{CO2,LT}}$ taken from the Takahashi climatology), but any such contribution is corrected for by adjustments to $C^{\text{DIC,}\Delta\text{ini}}$ in the inverse estimation.

Therefore, any of our target quantities is virtually independent of the GLODAP gridded product. We will reformulate the relevant sections to make this transparent in the paper.

The authors indicate that the SOCAT data was only used to improve the seasonal cycle (p 2279, line 15). I'm curious about how any underlying trends in the pCO2 data have been handled over the study period or whether any thought has been given to how much the smooth seasonal cycles predicted by the inversion could be biased by interannual variability.

Trend in parallel to the atmosphere are included explicitly through p_a^{CO2}, and deviations from that trend are also possible though the adjustable long-term component of the

ocean-interior flux (slightly larger/smaller ocean-interior flux than sea-air flux will lead to carbon accumulation/loss in the mixed layer over time).

However, developments during the publication and discussion phases of the paper made it possible to slightly update the scheme now, by also including interannual degrees of freedom to be adjusted by the data (corresponding changes have been made to the Methods section and Appendix A). It turns out that the mean seasonal cycles focused on here are hardly affected from this change, except for smaller changes in the North Pacific and in the Tropics. This confirms in retrospect that such effects from interannual variations are small even in the purely seasonal configuration.

I am also interested in seeing what the pCO2 residuals look like (val- ues predicted by the inversely estimated fluxes minus observations used to constrain the inversion) and if there is any spatial or temporal coherence in these residuals.

The residuals (especially their seasonal component) had been shown in the Supplement, Sect. S5.

In order to make them more visible, we moved part of this into the main text (new section "Fit to the data"), and added more references to the Supplement.

In section 4.5, the authors suggest that this could also be considered as a very sophisticated mapping tool for the pCO2 data. It is my understanding that pCO2 can change quite rapidly across fronts and other ocean features, whereas the method employed in this approach enforces a substantial degree of smoothing in space and in time through the a priori correlations described in section 2.4. Would the authors please comment on whether they see this as a limitation of this application.

Indeed, most of these small-scale features will not have been recorded by the available measurements and can therefore not be explicitly constrained in our scheme. It is also

the case that features resulting from small-scale internal fluxes cannot be reproduced by our scheme as the a-priori correlations damp them out. However, features related to temperature, or to effects of piston velocity variability, will be reproduced (to the extent allowed by the resolution and the realism of the driver data). Depending on the location, this will cover a large fraction of the real variability.

We added further validation figures, also using independent pCO2 data, to substantiate this (most of the new figures are placed in the Supplement to avoid further increase in paper length).

Appendix B: This synthetic inversion represents a good first step, but using a heavily smoothed synthetic dataset with only smooth interannual variability circumvents a lot of the issues that could cause biases in a real inversion. This should at least be discussed.

The same tests have also been done using daily process model simulations as "known truth" which involves also interannual and short-term variations. The performance of the diagnostic scheme is still very similar, confirming that the smoothness of the "known truth" used in the paper does not unduely help.

The reason not to use the test based on the model simulations was that this process model, while agreeing well with the pCO2-based results in the temperate and low latitudes, it is opposite in phase in the high latitudes.

The quality of the English and grammar was generally very good, but the manuscript (particularly the appendices) could benefit from a more thorough proof read prior to resubmission. Since I have requested substantial revisions, I have not noted specific cases in this review.

Detailed comments:

P. 2278, top: It could be quite useful to include a concise discussion of the atmospheric trans-

port model. How did it do in intercomparison experiments (e.g. Transcom)? What about evaluation against aircraft data (e.g. Stephens et al., 2007)?

As the most central result (run SFC) does not involve the atmospheric transport model, and several intercomparison studies in the community looked at such model evaluation anyway, we feel that such material would unduely lengthen the paper.

P. 2278, line 4: Including the references to Wanninkhof et al., 1992 and Naegler et al., 2009 (as well as in the appendix) would convey a lot of information to people who are familiar with these parameterisations without adding a lot of bulk to the paper.

This has been added as suggested.

P. 2278, line 12: It would be useful to include a short discussion here about how the authors expect the assumptions and approximations described here might affect the results. Are there good arguments to be made that effects would be small? Could they lead to biases? Is anything understood about whether the results would be biased high or low?

Many of the error influences are compensated by corresponding adjustments to the internal fluxes, and are therefore not affecting the estimated pCO2 field and sea-air flux much. We added more explanation on this, and more sensitivity cases to make it quantitative.

P. 2278, line 24: One of the principal advances of this inversion over previous methods is the inclusion of the SOCAT data. I would find it helpful to have here (or in the introduction) a little more information about the SOCAT dataset. How good is the spatial coverage of SOCAT? Where is it weak/strong? How do these data compare with the classical Takahashi climatology, which has been used to constrain inversions through priors for a long time? How much overlap is there in terms of the raw data included in each? What are methodological differences in how

the data have been compiled?

The SOCAT data have been compiled in a systematic/coherent way following agreed and fully documented procedures, including a quality control protocol. The input data used for (re-)calculating SOCAT fCO2 are publically available from the SOCAT website.

There is a large overlap between the data included in SOCAT and LDEO data sets. Both data sets have been mutually informing each other. SOCAT comprises substantially more data, including coastal data. It does not however include fCO2 calculated from e.g TA and DIC (only measured fCO2).

Much of this information is found in the cited SOCAT paper by Pfeil et al. (2012), including the distribution of SOCAT data per decade (their Figure 2) and data per latitude for the years 2000 to 2007 (their Figure 4). Data distribution had also been shown in our Supplement, including seasonal differences (Fig S7.4). Differenes between the Takahashi climatology and the SOCAT data points had been shown in the supplementary Sect. S5.

Sections 2.5.1 and 2.5.2: In both of these cases, it would be nice to have a concise summary of what was done and what the results were, even if the full details are in the appendix.

These two sections are now folded into the new Results and Discussion section "Data and model constraints", with some short summary as requested.

P. 2281, line15 on: This is where it would be helpful to have a deeper understanding of how independent the SOCAT and Takahashi datasets are. Are all the Takahashi data also included in SOCAT? If so, should we really be impressed about agreement between the two?

Not impressed, but relieved: The comparison to the Takahashi et al climatology was meant to ensure that those modes of variability common to both products –the seasonal

cycle and its spatial pattern– do agree to the expected extend, confirming that the results of both methods are informed by the data and not primarily method-dependent.

The effect of different underlying sets of data (SOCAT and LDEO, respectively) was addressed in the Supplement (Sect S6).

P. 2281, last two lines should be rewritten to improve grammar.

An "e" was missing in "note".

P. 2283, lines 23-24. This is similar to the finding of previous studies that included both oceanic and atmospheric data (e.g. Jacobson et al., 2007). This should be noted.

The similarity to Jacobson et al. had been referred to already, but we tried to make it even more clear.

A1.2: It would be helpful if the authors would start with a couple of sentences laying out the derivations that they are about to undertake, so the reader can see where they are going more easily.

This has been added.

Equation A6: I think a beta must have been accidentally left out here (it reappears in A7).

No, Eq (A6) denotes the reference point of the linearization, which does not depend on any of the actual driver fields. It does not contain beta which describes the deviation from this reference point in the temperature dimension.

A1.3: It would help guide the reader if the authors pointed out that fint is the quantity that is

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estimated by the inversion in the first paragraph.

We now mention that this section aims at estabishing mixed-layer concentration as a function of ocean-interior source/sinks. This is now also announced at the beginning of A1.

P. 2297, lines 5-9: Confusing sentence; please reword.

We re-wrote the paragraph.

P. 2298, lines 4-8: I was wondering if this history flux leads to dipoles in the time domain (for example, an over estimate at t=1 leads to a compensating under-estimate in t=2), or if the regularisation scheme corrects for this.

In the approximation where the history flux is always calculated from the climatology, it is just a fixed contribution not changed in the estimation. If the history flux would be correctly calculated from the actual DIC concentration, then memory effects from one year to the next, which also exist in reality, would indeed be possible.

P. 2302, lines 22-23 and P. 2303, line 12: I'm curious about why the spatial correlation length/time scales were changed and how the new values were chosen.

Some more general remarks on the choice of correlation lengths have been added to App 2.2.

P. 2303, Line 17: It's not clear to me that assuming an a priori fint=0 is the same as assuming that you "have no information on the internal fluxes". In the absence of data, the a posteriori tends to damp to the a priori value. So, aren't you really assuming that the fint is only a small

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modulation of equation A.16 with this prior? Or, perhaps I'm not fully understanding the method.

We added a more detailed explanation in which sense fint=0 means "no information" into this paragraph and into a new section in the Result section.

On the other remark, f_{int} is indeed a modulation of equation (A16), but it is by far not "small": In terms of pCO2, it even overcompensates the seasonality of the prior in many regions (high latitudes). This is also addressed explicitly now.

P. 2304, line 5: Please expand on "technical reasons"

Line 5 was just the introduction of the following sentences giving the technical reasons. We made this clear by adding a colon, and by reference to Tab 4.

Interactive comment on Ocean Sci. Discuss., 9, 2273, 2012.

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