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Biogeosciences Discussions

Interactive comment on "A novel method for diagnosing seasonal to inter-annual surface ocean carbon dynamics from bottle data using neural networks" *by* T. P. Sasse et al.

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Dear Editor,

Below follow comments on the manuscript: "A novel method for diagnosing seasonal to inter-annual surface ocean carbon dynamics from bottle data using neural networks" by Sasse et al.

We thank the reviewers for their thorough comments and constructive suggestions on our manuscript. In our response below, we first address the comments made by Referee 1 (anonymous), followed by comments made by Referee 2 (Sarah Mikaloff-Fletcher). We hope that the manuscript in its revised form will be accepted for publica-

tion in Biogeosciences.

- Anonymous (General comments): The real value of this work lies in the three great improvements over previous attempts:...The first is the fact that the SOM and MLR are combined into one modelling system...The second improvement over previous work is the global scale of this analysis...Finally, the results presented in this manuscript are thoroughly validated against a series of independent in-situ data sets.

OUR RESPONSE: Thank you.

- Anonymous (Criticism): Recommendation to incorporate some of the supplementary material into the manuscript to improve reading flow.

OUR RESPONSE: We have incorporated supplementary material detailing our robust forward MLR routine (Supp. E) in section 4.1, geographical constraints (Supp. I) in section 6.1.2 and identifying poorly constrained coastal (Supp. K) in section 6.3.

- Anonymous (Specific comment 1): Page 15330, line 3: sparse – change to still insufficient. In general calling the current coverage of carbonate system parameters sparse seems inappropriate. It's greatest ever, achieved with enormous effort and still increasing. Yes, it's still insufficient for several purposes. I would look at this wording throughout the manuscript.

OUR RESPONSE: In the manuscript we acknowledge that enormous effort has been invested into establishing the global carbonate measurement network. We also agree with the reviewer that a more tactful approach should be used to convey current limitations of the dataset. We have therefore changed wording on P15331, line 15, P15332, line 11, P15346, line 10, and that suggested by the reviewer on page 15330, line 3 to better convey global efforts.

- Anonymous (Specific comment 2): Page 15346, line 25: Please change the sentence to: For AT, the benefits of using SOMLO are much weaker, with deterioration of system's detection in some regions. Table 5b: Would recommend specifying negative

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improvement for Eq. Pac and North Atl. In both cases above the authors should name appropriate what they show.

OUR RESPONSE: We have change the sentence on page 15346, line 25 to: For AT, the benefits of using SOMLO are much weaker, with only a marginal global improvement by 6.7% (or 0.7 μmol kg-1) and even deterioration of detection in the equatorial Pacific and North Atlantic.

We have also specified negative improvement in Tables 5b and 7

- Anonymous (Specific comment 2): Page 15347, line 14: The word anomalies should be replaced by influences in my opinion. Authors exclude all coastal influences from their analysis and not only the anomalous coastal data.

OUR RESPONSE: In this section, we used the global independent test (GIT) residual errors to investigate the spatial skill of our model. We found that samples with the highest residual error are typically located in marginal seas with known biogeochemical complexity. It is for this reason we refer to these samples as anomalies. We have incorporated supplementary material K and reworded 'coastal anomalies' to 'anomalous coastal data' to clarify our approach.

- Sara Mikaloff-Fletcher (General comments): Overall, I found this to be an excellent statistical treatment of an important global issue: improving our understanding of the spatial and temporal distribution of carbon species in the surface ocean. However, while the paper was rich in explorations of the technique, its errors, and potential biases, I found it quite thin on discussion of the end result. For example, two natural figures to include would be a map of the predicted DIC and Alkalinity from this approach next to maps of these values from the GLODAP gridded data set, and then a Takahashi pCO2 map next to a map of pCO2 calculated from this approach. This could have been accompanied by discussion of what can be learned from the higher resolution information about these tracers. Discussion of the predicted seasonal cycle would have also been exciting

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OUR RESPONSE: We thank the reviewer for their kind comments and suggesting potential applications of our new approach. However, as the current manuscript focuses on introducing and testing our new approach, results of this nature will feature in many future and longer discussion papers.

- Sara Mikaloff-Fletcher (General comments): In the Introduction, the authors argue that their approach will help to address questions about inter-annual variability in the carbon cycle. This occurs in a few places, but especially P15333, paragraph 2. I agree that you will gain a wealth of information about spatial and seasonal variability from applying the algorithms developed here to World Ocean Atlas data. However, to the best of my knowledge, the World Ocean Atlas does not include information about inter annual variability. Please discuss what data would be used to look at this question or de-emphasize this point in the introduction.

OUR RESPONSE: It is correct that the World Ocean Atlas does not include information about inter-annual variability [Antonov et al., 2010; Garcia et al., 2010a; Garcia et al., 2010b; Locarnini et al., 2010], however, the World Ocean Database [Boyer et al., 2009] contains in-situ measurements of standard hydrographic parameters taken over many years. By applying our predictive model to this dataset will permit us to investigate inter-annual carbon variability in regions with sufficient temporal data coverage. Two changes were implemented to clarify this point: 1) we removed the word 'global' from the sentence on P15333, line 25, and 2) it was discovered that the Boyer et al. [2009] journal article was incorrectly titled as World Ocean Atlas Dataset. We have corrected the title to 'World Ocean Dataset' thereby removing any confusion. Furthermore, we have mentioned and referenced the World Ocean Atlas products on page 15333, paragraph 2, to clarify the distinction between the datasets used to investigate seasonal and inter-annual carbon dynamics.

Regarding the other mention on P15349, line 10, we stated that our model could be applied to the many long-term hydrological time-series stations available in the ocean to investigate inter-annual variability. In this instance, we referenced the manuscript of

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McNeil [2010] that discusses in detail some of these datasets. We therefore have not include additional information.

- Sara Mikaloff-Fletcher (General comments): There is a limited discussion of the complimentary efforts underway to use satellite and pCO2 data to map sea surface pCO2 (P15334, top). This should be expanded to discuss in more detail what has been done in this area, what the limitations of these techniques are, and what the SOMLO method contributes, and whether there is any scope for the two methods to complement one another. This could be discussed partly in the introduction and partly in the discussion/conclusions.

OUR RESPONSE: In this manuscript we are focusing on introducing and testing our new technique to capture mixed-layer CT and AT using bottle measurements. We therefore leave a detailed discussion comparing the satellite and underway pCO2 data-based approaches to a future manuscript presenting our pCO2 results.

- Sara Mikaloff-Fletcher (General comments): While it can be quite beneficial for some of the more technical aspects of the paper to be included in the supplementary material, I felt that in this case some of the material that was quite central to the paper was also included in supplements. In particular, I would recommend including all or at least part of Supplement E in section 4. The authors have included a short sentence meant to summarize Supplement E in section 4.1, but I have to admit that I could not understand that sentence until after reading the supplement. Likewise, a description of the geographic training parameters in Supplement I would have been helpful on page 15345.

OUR RESPONSE: We have incorporated supplementary material detailing our robust forward MLR routine (Supp. E) in section 4.1, geographical constraints (Supp. I) in section 6.1.2 and identifying poorly constrained coastal (Supp. K) in section 6.3.

- Sara Mikaloff-Fletcher (General comments): The authors developed a Global Independence Test (GIT), which is a quite clever way of evaluating the predictive capability

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of the dataset without using the same data that was already used to constrain the problem but also without sacrificing a large amount of the available data for the final fit. While I quite liked the approach, it wasn't quite clear to me from the equation provided in section 3 exactly how the RSE was calculated. From the description, I have the impression that each cruise is, in turn, excluded from the optimization and used to evaluate the fit. Is an RSE calculated for each cruise? If so, how do the authors combine the RSE's from each cruise to get one number? Or is the numerator in Equation 1 summed over all of the cruises?

OUR RESPONSE: It is correct that data from each cruise and time-series is, in turn, excluded from the dataset used to train the global model and subsequently employed to evaluate the fit. To then calculate the residual standard error (RSE) using Eq.1 on page 15337, we combine the independent predictions from either all, or a subset, of the cruises/time-series to provide the most accurate estimate of the models global, or regional, skill (i.e. the numerator is summed over all, or a subset, of the cruises). We have expanded the outline of our approach on P15337, paragraph 2, to clarify this point.

- Sara Mikaloff-Fletcher (General comments): The authors use time-series observations from two tropical stations, the Bermuda Atlantic Time-series and the Hawaiian Ocean Time-series (BATS and HOT) to constrain and evaluate their approach. It would be interesting to also test these results against the Munida time-series (1998 to present), which samples Subantarctic Surface Water, just South East of New Zealand [Brix et al., 2013; Currie et al., 2011]. This region is likely to experience quite different ocean biogeochemistry than the other sites that were tested and the time-series includes all the required measurements.

OUR RESPONSE: We agree with the reviewer that testing our approach within a range of biogeochemically diverse regions would provide powerful insights into the models skill. However, there exist only a few time-series stations (BATS, HOT and Munida) with sufficient temporal data coverage of carbon and complementary standard hydrographic

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measurements to apply this approach. Since we currently only have access to data from BATS and HOT we are unable to test our model at the Munida station.

- Sara Mikaloff-Fletcher (Specific comments): P.15330, line 11, No comma after ML$. P. 15330, line 19, comma after network. P. 15330, line 26, no comma after complex, but comma after Pacific on the following line. P15332, line 12, replace has with have P. 15333, line 7, no comma after Southern Ocean. P15335, line 17, no parenthesis around Tanhua et al., 2010. P. 15335, line 3, comma after (Fig. 1b). P. 15337, line 15, no comma after data P. 15337, line 21, algorithms should be algorithm's. P. 15339, line 18, gives should be give P. 15341, line 16, comma needed after SOM Pl. 15343, line 10, comma after GIT. Also, GIT has been previously defined and does not need to be re-defined again. P15345, line 28, no comma after "zone"

OUR RESPONSE: Thank you for your edits. We have incorporated all the above suggestions.

- Sara Mikaloff-Fletcher (Specific comment): P. 15335, line 13, be a bit more explicit about the quality consistency (e.g. the quality consistency needed to directly combine data measured from different labs.)

OUR RESPONSE: We do not believe there is a quality consistency requirement to combine data measured from different labs, and therefore cannot be more explicit on this point. We would like to emphasize that the purpose of this paragraph was to identify the existence of systematic differences between independent laboratory measurements and to outline the approach used to correct for this issue when combining the data. Since we feel this has been adequately achieved, no further details were included.

- Sara Mikaloff-Fletcher (Specific comment): P. 15335, line 19, please be more explicit about the methods used to remove questionable measurements.

OUR RESPONSE: We removed questionable data using the existing quality control

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flags based on World Ocean Circulation Experiment (WOCE) convention [Joyce and Corry, 1994]. We have expanded the discussion on P. 15335, line 20, to incorporate this information.

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