

We thank Referee #2 for the review of our paper; we have responded to all of their comments below.

Comments from the Referee are in *black*; our responses are in blue.

Referee #2: Review of “Deriving a sea surface climatology of CO₂ fugacity in support of air-sea gas flux studies” by L. M. Goddijn-Murphy et al., Ocean Science Discussion

The authors apply a statistical “Kriging” method for the analysis of the SOCAT surface water fco₂ dataset to provide climatological (1991- 2013) mean distribution of surface water fco₂ over the global oceans. Instead of the archived bulk water temperatures measured around 5-meters deep, they consider that the satellite based temperature data at the base of surface skin layer are of higher and uniform quality, and they correct the reported fco₂ values to the sub-skin temperatures. The global ocean surface water fco₂ data thus improved are processed with the Kriging method for spatial interpolation to yield mean monthly distribution over the global oceans. Their approach is new and demonstrates some success in the data rich areas (such as the North Pacific and North Atlantic).

Reply: We thank the reviewer for highlighting the novelty and success of the approach.

Revision in paper:

None

Referee #2: On the other hand, for the areas where no or few observations are available, the method yields distributions that are not consistent with established ocean observations including circulation and biogeochemical processes. In this manuscript, the authors simply present the results of their output from the Kriging analysis in a map form (often in a small postage size format), but fail to compare their results with the earlier published work and neglect to present the critical evaluation of their results in the oceanographic context. I would therefore advise major revision for this manuscript before it is accepted for the publication. My comments are listed below.

Reply: The primary focus of this paper is to re-analyse the in situ f_{CO_2} values for in situ SST to f_{CO_2} values for monthly grid-box mean values of subskin SST. The complexities of in situ SST measurements and the implications for f_{CO_2} (Section 1.2), and the use of satellite SST data (Section 1.3) are explained in detail, and a comparison between the SST datasets is given (Section 1.4). The re-analysed f_{CO_2} values, representing ‘true’ monthly grid-box means, are normalized to a reference year and spatially interpolated using ordinary block kriging to allow the re-analysed data to be used for global air-sea gas flux studies. However, this latter stage is not the primary focus of the paper.

Hence we have not compared the kriged results to other equivalent spatially and temporally interpolated datasets. We will clarify this in the revised version of the paper. We will also improve the presentation of the monthly maps by presenting seasonal maps, rather than monthly ones for all figures. The actual dataset allows the user to make the choice on the variance value, but we appreciate that showing all values in the paper could mislead the reader to the quality of the outputs.

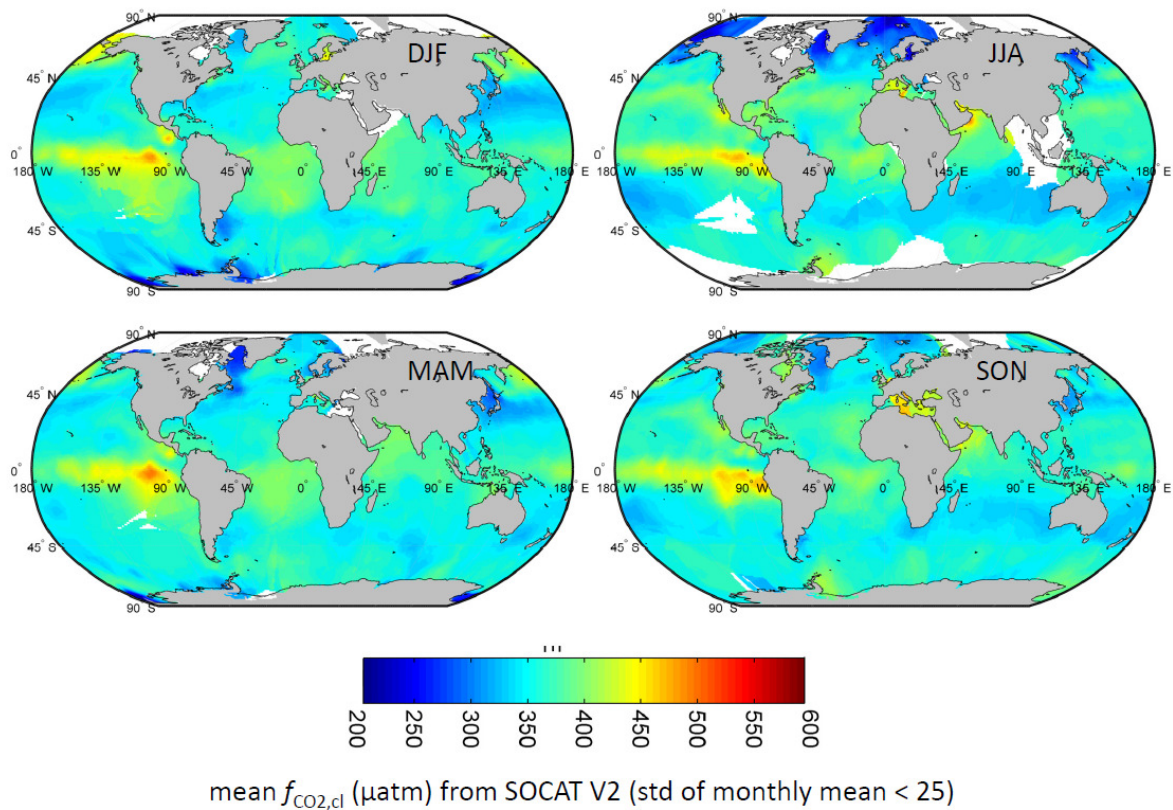


Figure R1. Mean $f_{CO_2,cl}$ (μatm) over the months, clockwise from top left, December to February, June to August, September to November, and March to May; only monthly mean values with std < 25 μatm were included.

Response in Paper:

We clarify the scope of the paper. We improve the choice and quality of figures (see reply to Referee#1 for changes to figures).

Referee #2: 1) Page 1900, Section 1.3:

The authors proposed that the sub-skin temperature has been measured with a uniform accuracy over the global oceans, and this should be used for obtaining seawater pCO₂ (or f_{CO_2}) rather than the bulk water temperature measured with questionable reliability. I agree with the authors.

Reply: Excellent. We are glad that the reviewer sees the scientific benefit of the work.

Response in Paper:

None

Referee #2: However, they fell short on explaining why it is more relevant to the sea-air flux of CO₂ studies than that at the skin-temperature. Sarmiento and Sundquist (1992, Nature) first pointed out that, for the estimation of the air-sea CO₂ driving potential, the pCO₂ at the skin-temperature should be considered rather than that at the bulk water temperature. Donlon et al. (2002, J. Clim.) observed that the skin-temperatures are on the average cooler than the bulk water temperatures measured at 5 meters deep by 0.17 ± 0.07 °C over the Atlantic and Pacific, 50°N-50°S. Also, the skin-temperature varies as much as 2 °C depending upon the time of day, season and weather conditions. The present authors should justify their reason for adherence to correcting the fco₂ to sub-skin temperature, rather than to the skin-temperature. I can recall two papers which address this issue. McGillis and Wanninkhof (2006, Marine Chem.) called attention to that the molecular diffusivities of CO₂ and salts in seawater are two orders of magnitude smaller than the thermal diffusivity. Therefore, the fco₂ difference between skin and sub-skin waters is negligibly small. Zhang and Cai (2007, GRL) pointed out that the skin cooling tends to be accompanied with increasing salinity, and hence, their respective effects on seawater fco₂ cancel each other. These studies support that the fco₂ at sub-skin temperature is a relevant quantity for the sea-air CO₂ flux studies.

Reply: Using any sub-surface temperature throughout the air-sea flux calculation is definitely wrong since the aqueous concentration at the top of the mass boundary will then be wrong (by about 2.7% / degree of temperature difference)

Following from the insights of McGillis and Wanninkhof (2006), it is arguable how the fugacity at the base of mass boundary layer should be calculated, since this will be within the thermal boundary layer. We stand by our choice of calculating fugacities corrected to a monthly-composite sub-skin temperature, firstly because of the quality of this temperature product, and secondly that it will in combination with a sub-skin solubility (calculated using the same temperature product) give an accurate estimate of monthly-composite concentration. In our view, concentration changes between the base of the thermal boundary layer and the base of the mass boundary layer are ambiguous, but small compared to other corrections.

Response in Paper:

None specific, but we review the explanations to bring extra clarity to the text.

Referee #2: 2) The authors should explain the “Kriging” method and justify its application for the interpolation of the SOCAT fco2 data. Fig. 1A shows that the standard deviations for April not only jump up suddenly but also their distribution changes suddenly from the adjacent months. In November, the standard deviation becomes, again suddenly, nearly uniform all over the global oceans including the polar oceans. In Section 5.2 (page 1914), the authors commented these features and provided short and unconvincing explanations. This issue should not be treated so lightly, that these features represent instability of the computational method used, and hence cast doubt on the reliability of the results. Although the authors refer to the variogram (Figure 4) for the explanation, Fig. 4 is difficult to read and understand (the values and axes are not readable because of poor reproduction). While the surface ocean fco2 and many other properties are known be distributed in distinctly zonal belts, the variogram does not appear to show these distinct trends representing the zonal structure. The authors are requested to explain how the variogram influences the results.

Reply: To allow the re-analysed f_{CO_2} data to be used for global air-sea gas flux studies we apply a simple kriging result to produce spatially complete fields along with an estimate of the error in the kriging. However, this stage is not the primary focus of the paper. We will improve the presentation of the monthly maps by presenting seasonal maps, rather than monthly ones for all figures (e.g, Fig. R1). We will also only display data that pass a specified variance quality value, so that regions with large errors are not visible. The actual dataset allows the user to make the choice on the variance value, but we appreciate that showing all values in the paper could mislead the reader to the quality of the outputs. The kriging method is deliberately simple as i) it is not the primary focus of the paper but enables others to exploit the data, ii) the kriging provides an error estimate of the predicted values, and iii) there is at least international effort studying the effects of different spatial and temporal interpolation schemes and this is a whole area of research in itself and well beyond the scope of this article.

We will add more information about the method and the variogram, also adding a reference to the technique (Pebesma 2004). To help clarify the method Fig. 4 will be updated (see below)

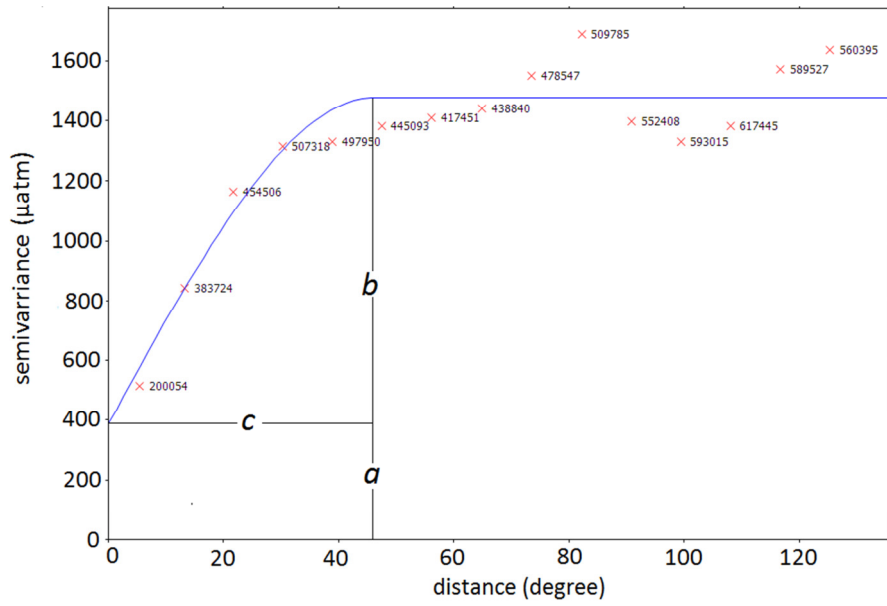


Figure 4. Variogram for global $f_{CO_2,cl}$ data in 2010 for the month January, derived from $f_{CO_2,is}$ shown in Fig.3. The numbers next to each data point are the number of data pairs.

and the following text will be added on page 1910, Line 22, after “... (e.g., Fig. 4):

“Fig. 4 shows that at small separation distances, the semivariance in f_{CO_2} (computed as one half the difference in f_{CO_2} squared) is small so that points that are close together have similar f_{CO_2} values. After a certain level of separation (c), the variance in the f_{CO_2} values becomes rather random and the model variogram flattens out to a value corresponding to the average semivariance ($a + b$). The model variogram is used to compute the weights used in the kriging. The variogram coefficients were different for each month because each monthly dataset had a different data distribution.”

We would like to note that the variogram results from the geospatial data itself. To further highlight the deliberate use of a simple interpolation method we propose to replace Page 1911, Line 21-22 , “The spatial interpolation ... unbiased results (Pebesma, 1999).” with “By using the variogram to compute the weights for the interpolation, the expected estimation error is minimized in a least squares sense. For this reason, kriging is expected to produce the best linear unbiased estimate.” Admittedly, other more complicated and specialised interpolation schemes may provide more visually compelling spatial fields, but they would require a priori knowledge of the distribution of f_{CO_2} . As this was not the main focus of the work we chose to minimize the expected error in a least squared sense without using a priori knowledge to produce a simple but useable result and we leave the development and analysis of more advanced schemes to other research studies. Using the spatial fields of standard deviation the user can decide what level of uncertainty is acceptable for

their specific application allowing them to exclude those grid boxes or use only areas of high data density.

Response in Paper:

Several changes as outlined in the reply above.

Referee #2: 3) The authors cover the entire global ocean areas with the results of Kriging extrapolation. However, in a number of areas, the Kriging results are inconsistent with the established oceanographic knowledge. For example, the Antarctic Circumpolar Current (ACC) is a zonal current system that forms a well defined frontal structure abutting the subtropical waters to the north. Although the ACC waters are transported northward via eddies, earlier studies show no indication for cross-frontal meridional currents as suggested by the N-S structures shown in Fig.12 and 13. I presume that these features are caused by the sparse and seasonally biased observations. Also, some narrow but distinct features (such as seasonal intense upwelling along the Chilean west coast and Arabian Sea) are not shown in these figures. Again, the missing features are due to the absence of observations. The authors pay little attention to the part of the oceans covered with permanent or seasonal ice covers, and provide indiscriminately values for these areas. There are no or little observations in the ice field waters. I would therefore suggest that, although the Kriging gives values for the areas with poor or no data coverage, these areas should be left blank, because the credibility of the good reliable results may be eroded by the inclusion of these oceanographically unreasonable values. Although the authors claim that the Kriging method yields “unbiased” results, they should exercise a proper degree of oceanographic “bias” to their results.

Reply: As explained above, more complicated and specialised interpolation schemes may provide more visually compelling spatial fields but they would require a priori knowledge of the distribution of f_{CO_2} . We will briefly discuss other interpolation techniques and compare the applied methodologies but we will not compare their results as this was not the main focus of our work. We chose to minimize the expected error in a least squared sense without using a priori knowledge to produce a simple but useable result and we leave the development and analysis of more advanced schemes to other research studies. Naturally in areas with low data density the kriging errors were big but at least they could be quantified in an objective manner. To aid the user, the expected error in the kriging prediction at each interpolation point is given so that the user can decide what level of uncertainty is acceptable for their specific application.

Response in Paper:

The scope of the paper is clarified. We add some brief discussion of other methods and studies as outlined in the reply above.

Referee #2: 4) Throughout this manuscript, the graphic presentation for the global distribution should be improved to make the maps more formative in the oceanographic context. For example, the distribution of fco2 in the Pacific is broken in the middle (Figs. 5, 12 and 13 and many other postage-stamp-size world ocean maps), so that the unique features in the Pacific (including the equatorial El Nino zone, the Kuroshio, the Bering Sea and the Ross Sea) are not clearly demonstrated. I may suggest that either the prime meridian is shifted to accommodate the whole span of the Pacific, or the maps be expanded to encompass 450 degrees longitude ($360^\circ + 90^\circ$). The maps should not be forced into a square shape dictated by the computer software. At least, the authors try to present their fco2 results in the same map format used by the distribution of data and errors (e. g. Figs.3, 9, 10, 11 etc), so that the readers can see the relationships between the observations and the distributions of fco2 and errors.

Reply: We agree that it is hard to display the results for each month within an A4 paper. We will re-format the spatial data for the paper into a pseudocylindrical projection as used by other authors and manuscripts. We will also convert the majority of the figures to represent seasonal representations (ie reducing the figure size from 12 monthly images down to 4 seasonal images). Following Rödenbeck et al. (2013) we centred the maps on 0° . This was so we could give optimal view on the North Atlantic because data quality was the best in the North Atlantic and many of the previous studies have been in the North Atlantic (Schuster et al. 2008; Landschützer et al. 2013; Watson et al. 2009).

Response in Paper:

We improve the choice and quality of figures (see reply to Referee#1 for changes to figures).

Referee #2: 5) *The postage-stamp-size maps are too small to see any details (e. g. Fig. 5). Although the January distribution is shown in a large format, this does not help to show major seasonal changes. Therefore, the authors should consider showing a pair of February and August maps, and discuss the seasonal changes, especially the phase differences between the seasonal changes in the sub-polar and temperate oceans. Furthermore, since fco2 will be used for the computation of the sea-air CO2 flux, its global distribution should be best presented in an equal-area (or semiequal area) projection maps rather than the Mercator or other projections, which greatly distort the areas of high latitudes.*

Reply: As described above, we agree that it is hard to display the results for each month within an A4 paper. We will re-format the spatial data for the paper into a pseudocylindrical projection as used by other authors and manuscripts. We will also convert the majority of the figures to represent

seasonal representations (ie reducing the figure size from 12 monthly images down to 4 seasonal images, Fig. R1).

Response in Paper:

We improve the choice and quality of figures (see reply to Referee#1 for changes to figures).

Referee #2: 6) In page 1908, Section 3.1, Inversion of fco2 to pCO₂, the authors present lengthy and contorted computational procedures for converting fco2 to pCO₂ to salvage the SOCAT listings, which only gave fco2 values but no other relevant data such as Xco2 (dry or wet) or pCO₂. In their summary in Section 5.6 for Inversion Error, they conclude that the bias from the inversion is minor. In view of this finding, they should eliminate the contorted presentation in Section 3.1 totally, and replace it with a brief summary of their findings.

Reply: This is a good point and we will replace those lengthy sections with a brief summary as suggested and move the details to the appendix.

Response in Paper:

Revision of structure as described above.

Referee #2: 7) While shortening of Section 3.1, the authors should expand the analysis of their fco2 product in the oceanographic context. For example, zonal mean values may be plotted as a function of longitude or month to show the meridional and seasonal variability in three major ocean basins.

Reply: The scope of our paper is deliberately limited and we do not want to extend the paper to discuss any oceanographic implications. Our intention is to make available a new dataset prepared with clearly stated assumptions that we and others can use alone or in comparison with comparable data sets calculated under different assumptions. We appreciate that the oceanographic analysis may be more interesting to many readers than our presentation of the motivation, methods and results, but we think that this paper stands on its own merits.

Response in Paper:

The scope of the paper is clarified. No specific changes.

Referee #2: 8) Pages 1903- 1909: Various “temperatures” (T, Teq, SST,...) in different scales (Celsius and Kelvin) are used in equations. Please clarify the confusion. Would T(K), T(C) work?

Reply: In equations (1)-(4) temperatures are in kelvin (see page 1905, Line 5-6). We will double check the whole manuscript for any missing temperature units.

Response in Paper:

Units are added where missing.

Referee #2: 9) Page 1903, line 18: Change to “.... To reference year 2010 using a simple linear relationship with a mean increase rate of 1.5 ± 0.3 uatm yr⁻¹”.

Reply: yes, we will make the change as suggested.

Response in Paper:

Corrected as suggested

Referee #2: 10) Page 1904, Eq (1) and (2): The authors cited Weiss (1974, Marine Chem.) for Eq (2), but did not cite Eq (1), which was determined by Takahashi et al. (1993, GBC).

Reply: OK, thank you. We will add the appropriate reference. (Takahashi et al. 1993)

Response in Paper:

Corrected as suggested

Referee #2: 11) Page 1906, Line 12: The left side of the equation should be “partial differential” (for constant chemistry), rather than “total differential” (Takahashi et al., 1993, GBC). Here T is in °C.

Reply: In the PDF that we have viewed the equation is a partial differential ($\delta/\delta T$), so we suspect that the problem the reviewer has seen may be related to their PDF viewer and its font settings.

Response in Paper:

Formatting will be checked.

Referee #2: 12) Page 1911, Line 6, Fig. 4 and Table 2: What are the unit for the min, max and radius numbers? Is it 1° x 1° pixel numbers? What is the unit for Distance in Fig. 4 horizontal axis? What is the vertical axis (can not read)? Is it a Kriging parameter? Please define.

Reply: We apologise.

Response in Paper:

We will add the definitions and units as specified.

Referee #2: 13) Page 1916, Lines 16 and 17: Add °C to ± 0.17 and ± 0.1 .

Reply: OK, we will clarify the units.

Response in Paper:

We will add the units as specified.

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