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Interactive comment on "Comparison of seven packages that compute ocean carbonate chemistry" *by* J. C. Orr et al.

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Response to Short Comment by Dr. Lisa Robbins

This Short Comment is repeated below in gray; our response follows in black.

Orr et al. have done an admirable and thorough job comparing calculation packages for carbon, which is a real service for the community of users. They have set forward useful recommendations for developers that should provide enhanced reproducibility for users.

We thank Dr. Robbins for sharing her view on the utility of this study.

With respect to CO2calc, we have a few comments and edits for the manuscript: At line 24-25, the authors note that: "Our early findings led developers to update two of those packages, seacarb and CO2calc" it is unclear to the reader whether the analysis presented here reflects those updates, which for CO2calc, does not. The particular problems that were revealed relate to a coding error specific to the Lueker calculation. This error was immediately corrected and the updated version of CO2calc (1.2.9 and later) can be found at http://pubs.usgs.gov/of/2010/1280/. This is the primary link for CO2calc and should be reflected in the manuscript.

In the revised manuscript, we will make it clearer that the text and figures reflect the most recent results from CO2calc as well as the other packages. The only exception will be the figure where we show results from older versions, some of which deviate significantly. The revised manuscript will also provide the URL mentioned above as the reference for CO2calc.

In Table 11, the pK1, pK2 and pKB values are incorrect for CO2calc. The actual pK1 and pK2 values for the Table 11 should be: 5.84715289, 8.96595149, and 8.59697, respectively. We believe these discrepancies stem from the fact that the authors calculated the various equilibrium constants based on output data rather than with the source code (although the source code has always been available on request). Because the output values do not have enough significant figures to back calculate the K values, the resulting values provided in Table 11 erroneously produced an artifact of high variability for pH (the increased variability about the mean noted by the authors in section 3.2.3) and many of the other parameters, as illustrated in the figures. The precision for pH output in CO2calc is limited to 3 decimal places for pH, and does not reflect the internal calculations that use pH in the CO2calc calculations. However, this finding does suggest that, for users that are likely to use CO2calc pH output in future

calculations, CO2calc output for pH should be increased to 6 decimal places. We also found that a short-hand description of the Mojica Prieto and Millero (2002) constants in CO2calc lacked information, and therefore, will be adding the correct reference for these constants.

In the submitted manuscript, we did point out the same probable cause of the variability for CO2calc's pK_1 and pK_2. It is nice to have that confirmed by the CO2calc developers. We are still considering how to change Table 11. For consistency, we wish to provide only the results from our analysis, not from what any of the developers has come up with on the side. This problem could be resolved though if the CO2calc developers would provide a new public version with more significant figures in some of their output variables, including pH. Even better would be a new version where values of the equilibrium constants were also made available to the user. Of course, any other improvements, such as that mentioned concerning documentation would be welcomed, even if not critical to our analysis.

We will stand by our usage of the Millero (2010) calculations using the K2 as provided by Millero until a resolution is determined.

Given the discrepancies identified by our Discussion paper, it seems that if a user would choose to employ the Millero (2010) K_1 and K_2 constants, the best bet would be to calculate them with the unpublished set of coefficients that Millero provided personally to CO2calc developers. However, the discrepancies between the results when using different sets of coefficients are large. Until Dr. Millero himself addresses this issue, we consider it premature to use the Millero (2010) constants with any set of coefficients. We think that even some of the unpublished sets may lack sufficient precision, as pointed out in the manuscript.

We suggest that editing the plots will make the paper more "readable", using unique colors and/ or symbols to represent the programs. Also use consistent symbols representing the programs between the figures. Without zooming into the plots, the symbol and color for some programs were easily mistaken for another. One small typo is noted at the top of the Figure 5: "Salinity" is misspelled. Otherwise the manuscript is very well written.

In the revised manuscript, we will strive to make the plots clearer. The above-mentioned spelling error will be corrected. Many thanks for these comments and the advice.

Interactive comment on Biogeosciences Discuss., 11, 5327, 2014.