

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

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Received and published: 13 May 2014

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.

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.

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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 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.

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

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.

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