

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. Jean-Pierre Gattuso

The Short Comment from Dr. Gattuso is repeated below in gray; our response follows in black.

Orr et al. (2014) identified bugs in the R package seacarb, which had very little effect on computed results when used with the best practices constants (Dickson et al., 2007), and highlighted very long processing time on big data files. Version 3.0 has just been released and can be downloaded from CRAN. The package has been modified to fix the minor bugs and optimize the code, leading to a dramatic increase

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in speed (35x to 50x faster). See the change log for more details. Note that there remains an issue with the formulations of the two dissociation constants of carbonic acid, K_1 and K_2 , from Millero et al. (2010). This issue should be resolved soon and seacarb updated accordingly. In the meantime, it is suggested to refrain from using this formulation in seacarb.

As always, any bug report and suggestions are welcome (gattuso(at)obs-vlfr.fr).

Change log, version 3.0, 2014-03-06

1. Major update led by Jean-Marie Epitalon, who has become a coauthor of the package.
2. Speed optimisation of the computation of dissociation constants by (1) using vectors rather than loops and (2) passing optional parameters. The increase in speed is up to 35x.
3. Computation of dissociation constants:
 - One or two pHScale conversion factor(s) are passed as optional parameter(s) to speed-up computation: (i) kSWS2scale to convert from the seawater scale (SWS) to the pH scale selected at the hydrostatic pressure value indicated and (ii) ktotalsWS_P0 to convert from the total scale to the SWS at an hydrostatic pressure of 0. These conversion factors are calculated using function kconv() if they are not given.
 - Computations are vectorized rather than using loops.
 - Warning messages for out-of-validity-domain: only one message per constant (instead of one per data entry).

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4. Pressure correction function Pcorrect:

- Two pHScale conversion factors are passed as optional parameters to speed-up computation: (i) kconv2Scale to convert from the pH scale selected to the SWS (or free for Kf) scale at the hydrostatic pressure value

We thank Dr. Gattuso for this notification of improvements to the seacarb package, notably its dramatic acceleration, and hope along with him for resolution of the discrepancies between Millero's (2010) different sets of coefficients for K_1 and K_2 . In the revised manuscript, we will update the text and figures with results from the latest version of seacarb.

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