

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

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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 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

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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).
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

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indicated and (ii) `kconv2ScaleP0` to convert from pH scale selected to the SWS (or free for `Kf`) scale at the hydrostatic pressure value indicated. These conversion factors are calculated using function `kconv()` if they are not given.

- Computations are vectorized rather than using loops

5. pH scale conversion `kconv`:

- Two dissociation constants passed as optional parameters to speed-up computation: `Ks` and `Kff`, which is `Kf` on the free pH scale

6. All these optional parameters not only allow faster calculations, they also allow more precise computation since the pHscale conversions are now based on the `Ks` and `Kf` values calculated as selected by the user (Dickson or Khoo for `Ks`, Perez & Fragra or Dickson & Goyet for `Kf`). In a previous version, an attempt has been made to remember `Kf` formulation choice but it does not support the case of data set with different choice for each entry.

7. carb function:

- Instead of looping through data: processing is made in batches
- For each particular value `f` of flag, a subset of all data is created based on `flag=f`, then this subset is processed in one shot
- When the Taylor approximation algorithm is used (call to `uniroot()`), a loop iteration over data is still used
- Dissociation constants `Kxy`: for each `Kxy`, a vector of values for all data is computed at the beginning in one shot; there is only one call to the function `Kxy()`
- When `flag=8`, the approximation of DIC by the Taylor algorithm is replaced by direct computation as DIC is linearly dependent on carbonate alkalinity.

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8. buffer function: computations are vectorized rather than using loops.
9. Kf now uses a correct formulation for ionic strength.

References cited

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