

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

Dr Olafsson (Referee)

jon@hafro.is

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Jón Ólafsson (Referee) jo@hi.is, jon@hafro.is

General comments

A bit over two decades ago there was no publicly available software for the calculation of sea water carbon chemistry parameters. A few gurus had developed their own programmes. There was also lively debate on the reliability of the different literature sources for the carbonic acid dissociation constants. The choice of analytical methods for sea water carbonate chemistry and best analytical practices were a matter of different groups or schools. The situation is very different now due to efforts generated within the oceanographic community and for individual or team efforts that have

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provided invaluable service to this community.

In 1998 Lewis and Wallace made publicly available the CO2SYS software for carbonate chemistry. It provided several options for input and output choices of conditions and of thermodynamic parameters. CO2SYS was thoroughly documented. Currently there are six additional publicly available packages for the computation sea water carbonate chemistry. The paper under review here is important for the chemical oceanographic community and anyone who studies the sea water changes that are driven by anthropogenic releases of carbon dioxide. The sea water carbonate computation packages have applications in global models on mainframe computers, on personal computers and who knows, the youth you see busy with an iPhone may be checking on aspects of future ocean acidification.

This is a timely contribution. The comparability of the computation packages has been an open and important question in discussions on different data evaluations. Another application of the software packages is in chemical oceanography education and training.

In this paper the basis for the comparison tests is clearly described and the different results of the comparisons are also clearly presented. The authors explain the comparison results and outline where there is safe ground to tread. They also give attention to recently emerging issues, such as that of boron alkalinity and to the long standing questions on the carbonate system in low salinity waters. There the authors have devoted a thorough effort to explain observed differences between the software packages when applied to the low salinity range. Finally the authors provide several recommendations for software developers and users. No doubt, this work will also lead to improved versions of the currently available carbonate computation packages.

Conclusion

This reviewer is a user of sea water carbon chemistry software who finds this work an admirable service to the community and welcomes its publication in Biogeosciences.

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