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Interactive comment on "Improved routines to model the ocean carbonate system: mocsy 1.0" *by* J. C. Orr and J.-M Epitalon

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Response to Comments by Referee 3

We thank Referee 3 for his comments, which are repeated below in gray; our responses follow in black.

Summary

The manuscript presents a revised and updated oceanic carbonate chemistry scheme, MOCSY, intended for use by both observational scientists and carbon cycle modellers. Updates include a number of amendments to existing schemes, some new parameterisations and a general effort to permit a range of possible inputs that will suit most researchers (e.g. units, in situ vs. potential temperature). The manuscript also includes

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instructions to allow readers to download the scheme.

Overall, the manuscript is clear and well-written, though I have a number of minor criticisms described below. The associated Fortran code is easy to access, compile and run, both with the included test case and as part of custom code (essential if it is to be adopted by modellers).

Please note that I am a user of carbonate chemistry calculators like MOCSY rather than a chemical oceanographer. As such, my comments deal more with use of MOCSY than its fundamentals.

Specific comments

The following are minor comments relating mostly to edits that may slightly improve the manuscript. They are followed by a few remarks concerning my experience building and running MOCYS.

Pg. 2878, ln. 28: Careless readers (such as this one) may misinterpret "nutrient contributions" to refer to the consequences for proton concentration (and thus pH) of the use of nitrate and ammonium by phytoplankton; probably later rather than here, a "not-to-be-confused-with" statement might head this off

An excellent point. We will add such a statement in the revised manuscript.

Pg. 2879, ln. 7: "In many models ..." – it might be helpful if the authors gave a few examples, more so that readers are aware of the diversity of uses to which the OCMIP code has been put; citing examples of use of the code by OCMIP itself might be useful too

We will add some references to the end of this sentence in the revised manuscript.

Pg. 2881, ln. 3-4: "... from only one input pair ..." – this is slightly confusing because the code makes use of other inputs (which are mentioned later); perhaps this needs to be qualified with a specific reference to these being carbonate inputs – my reading

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of this is the authors are hinting at possible (but unstated) alternative inputs that are sometimes used to constrain the carbonate system (e.g. pH)

In the revised manuscript, we plan to change this potentially confusing sentence into 3 sentences: "Fortunately the ocean carbonate system is well constrained so that any pair of carbonate system variables can be used to compute all others when also given temperature, salinity, and nutrient concentrations. Yet unlike other public packages, mocsy is designed for models. Thus it offers users only one input pair of carbonate system variables, C_T and A_T, from which to compute all others."

Pg. 2883, ln. 26: "[HF]" is not defined; please make sure that all chemical terms are defined when first used (or, probably better here, in a table); this work will likely be used by non-specialists involved in carbon and climate research and it is important that they are not waylaid by abbreviated terms that they are unfamiliar with

In the revised manuscript we will mention that [HF] means hydrogen fluoride.

Pg. 2884, section 3.1: the authors present this section almost as a "disagreement" between "gentlemen models" and do not make it clear whether one model is better or worse than the other; perhaps this cannot readily be assessed to the required accuracy, but the authors could simply say so if this is the case

In the revised manuscript we will clarify that there is no absolute reference when it comes to computed carbonate system variables. Both packages could in principle be wrong even if both agree. However we compare mocsy to CO2SYS because the latter is the first public package made available to compute these variables, it was developed with great care (Lewis and Wallace, 1998), and it is used widely. Our companion manuscript goes into more detail about why we arbitrarily chose CO2SYS as the reference (Orr et al., 2014).

Pg. 2885, section 3.2: this section refers, correctly, to the errors caused by making the assumptions mentioned, but associated figure 3 instead presents these errors in the

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context of “corrections”; the implication being that one could keep using the approximations and just adjust the answers appropriately – surely we don’t want people to do this?; it would be better if the paper was consistent in its branding of these differences as errors to be avoided (by, for example, using mocys-1.0!)

For the revised manuscript, we are considering remaking these plots, showing the errors directly, not the corrections.

Pg. 2885, ln. 25: as the authors present the magnitude of errors or differences elsewhere I would expect them to give some notional (quantitative) idea of why the differences caused by the Kf option can be neglected

Because K_F is used only to convert between the seawater and total pH scales, and the difference between the two is small ($\sim$0.01 units of pH), for all intents and purposes the computed carbonate system variables are insensitive to changes in K_F. We will mention these details in the revised manuscript. We will also refer the reader to the sensitivities of computed variables to each constant that are shown in our companion paper (Orr et al., 2014, Table 9).

Pg. 2886, ln. 2: “substantial differences” caused by 1. total boron and 2. K1 and K2 are both mentioned here, but while numbers are presented in the following paragraph for boron, K1 and K2 go unmentioned; is Figure 4 doing all of the talking?; a clarifying remark might help

In the revised manuscript, we will add a brief discussion on the differences in K_1 and K_2 shown in Fig. 4.

Pg. 2886, ln. 3-4: is this tantamount to saying that models using the GLODAP climatology of alkalinity are effectively setting the oceanic inventory of this property wrongly?; I’m sure that I’m misreading that, but it may give readers this idea

No, this interpretation by Referee 3 is not what we meant to say. We appreciate the question though, because it does raise a flag for potential misinterpretation. The total

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alkalinity A_T in the GLODAP climatology is based on measurements of total alkalinity. If on the side we decide to calculate the individual contributions to alkalinity (A_C, A_B, A_W etc) using equilibrium constants and total concentrations (other measurements) that does not affect the total measured alkalinity. In the revised manuscript we will elaborate to avoid this potential confusion.

Pg. 2888, ln. 19-22: given the strong linear correlation between dissolved inorganic nitrogen and dissolved inorganic phosphorus, models that include N but not P could use a Redfield-scaled N as a substitute for P; this is likely to be a temptation for a number of models and this may be something that the authors could comment on here

This is a fine idea. It would allow a modeler to approximate the alkalinity from total dissolved inorganic phosphorus from the modeled total dissolved inorganic nitrogen. Unfortunately, we cannot use the same approach to approximate the alkalinity from total dissolved inorganic silicon. We will mention this potential partial solution in the revised manuscript.

Pg. 2890, Code availability: I would imagine that mocsy performs – in a computational sense – similarly to previous iterations (or rival packages), but it would be useful if the authors reported on any comparisons that they have made on it; for instance, does it typically converge in the same number of iterations?; I would expect so, but the additions to the complexity of the modelled chemistry may impact on this; one of the main groups of scientists who will be interested in this are ocean biogeochemical modellers, and reassuring them that the code performs comparably to what they currently use would doubtless help with its uptake by the community

The complexity of the chemistry in mocsy is identical to that agreed upon for the Ocean Carbon Cycle Model Intercomparison Project (OCMIP, Phase 2). In addition, it also computes the full suite of carbonate system variables, but that is not costly. We expect that the computational time of mocsy 1.0 is similar to that for the OCMIP2 code, but we have not tested it. On the other hand, for the costliest part of the code we have recently

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implemented a much improved approach, a new cubic initialization scheme combined with a more robust solver of the Alkalinity-pH equation, both from Munhoven (2013). With these improvements, mocsy 2.0 is up to 5 times faster. More details are provided in our response to another Referee of the manuscript, Guy Munhoven. The revised manuscript will present this new version of the code and discuss its improvements.

Pg. 2897, figure 3: the legend is ambiguous about the identity of the black dotted line; panel 1 labels it up, but it wouldn't hurt if the legend did too

In the legend to Fig. 3 in the revised manuscript, we will add: "Also shown is the sum of the three effects (black)."

Experience with code:

- Code successfully downloaded via OCMIP5 website (git has passed me by)
- Code initially failed to compile using ifort ...

```
sw_adtg.f90:11.19:USE msingledouble

1     Fatal Error:  File msingledouble.modópened at (1) is not a
GFORTRAN module file
```

- However, switching to gfortran in the makefile fixed this and was successfully able to build `test_mocsy`; the above error is most likely caused by local environment configuration
- `test_mocsy` successfully runs producing sample output for "model" and "observational" test datasets; I was also able to easily incorporate it within an existing Fortran subprogram ready for adoption within our local BGC model

Thank you for this feedback about your experience with the code. We have had no problem compiling and running it with either the `ifort` or `gfortran` compilers, nor

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have others that we have been in contact with. We are happy to hear that it could be included easily in your ocean biogeochemical model.

References

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Interactive comment on Geosci. Model Dev. Discuss., 7, 2877, 2014.