



**Model routines for
ocean CO₂ chemistry**

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Improved routines to model the ocean carbonate system: mocsy 1.0

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Abstract

Software used by modelers to compute ocean carbonate chemistry is often based on code from the Ocean Carbon Cycle Model Intercomparison Project (OCMIP), last revised in 2005. As an update, we offer here new publicly available Fortran 95 routines to model the ocean carbonate system (mocsy). Both codes take as input dissolved inorganic carbon C_T and total alkalinity A_T , the only two tracers of the ocean carbonate system that are unaffected by changes in temperature and salinity and conservative with respect to mixing, properties that make them ideally suited for ocean carbon models. With the same basic thermodynamic equilibria, both codes compute surface-ocean $p\text{CO}_2$ in order to simulate air–sea CO_2 fluxes. The mocsy package goes beyond the OCMIP code by computing all other carbonate system variables (e.g., pH, CO_3^{2-} , and CaCO_3 saturation states) and by doing so throughout the water column. Moreover, it avoids three common model approximations: that density is constant, that modeled potential temperature is equivalent to in situ temperature, and that depth is equivalent to pressure. These approximations work well at the surface, but total errors in computed variables grow with depth, e.g., reaching $-8 \mu\text{atm}$ in $p\text{CO}_2$, $+0.010$ in pH, and $+0.01$ in Ω_A at 5000 m. Besides the equilibrium constants recommended for best practices, mocsy also offers users three new options: (1) a recent formulation for total boron that increases its ocean content by 4 %, (2) an older formulation for K_F common to all other such software, and (3) recent formulations for K_1 and K_2 designed to also include low-salinity waters. More total boron increases borate alkalinity and reduces carbonate alkalinity, which is calculated as a difference from total alkalinity. As a result, the computed surface $p\text{CO}_2$ increases by 4 to $6 \mu\text{atm}$, while the computed aragonite saturation horizon (ASH) shallows by 60 m in the North Atlantic and by up to 90 m in the Southern Ocean. Changes due to the new formulation for K_1 and K_2 enhance $p\text{CO}_2$ by up to $8 \mu\text{atm}$ in the deep ocean and in high-latitude surface waters. These changes are comparable in magnitude to errors in the same regions associated with neglecting nutrient contributions to total alkalinity, a common practice in ocean biogeochemical

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modeling. The mocsy code with the standard options for best practices and none of the 3 approximations agrees with results from the CO2SYS package generally within 0.005 %.

1 Introduction

To compute air–sea CO₂ fluxes, ocean carbon cycle models compute the partial pressure of carbon dioxide ($p\text{CO}_2$) from two passive tracers, namely dissolved inorganic carbon C_T and total alkalinity A_T . In many models, that thermodynamic calculation is based on documented code from the Ocean Carbon Cycle Model Intercomparison Project (OCMIP), which is publicly available at <http://ocmip5.ipsl.jussieu.fr/OCMIP/>. Although modified versions of that code are used widely, it has not been updated since 2005. Meanwhile, there have been developments in recommended community standards for equilibrium constants (Dickson et al., 2007; Dickson, 2010).

Models require computationally efficient routines that are compatible with other model components, typically written in Fortran. Hence, model simulations are not made with widespread publicly available software packages that are designed to compute other carbonate system variables from any pair, given corresponding in situ temperature, salinity, pressure, as well as phosphate and silicate concentrations (Dickson et al., 2007). Models also differ because they typically carry potential temperature θ , use concentration units of mol m^{-3} , and are referenced to depth (m); conversely, equations for carbonate system thermodynamics require in situ temperature T , concentrations in mol kg^{-3} , and in situ pressure. Unit conversion is straightforward, but for simplicity modelers often make three approximations: (1) that θ is equivalent to T , (2) that ocean density is constant (e.g., 1028 kg m^{-3}), and (3) that depth (m) is equivalent to in situ pressure (dbar).

The errors associated with these simplifications are considered to be negligible, while the reasons behind them are largely historical. Most studies with ocean carbon cycle models have focused on large-scale patterns of air–sea CO₂ fluxes and

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related near-surface changes in the open ocean. More recently, with growing concern for ocean acidification (Caldeira and Wickett, 2003; Orr et al., 2005), attention has also turned to the deep ocean, the high latitudes, and local impacts in the coastal zone. Errors associated with the three approximations may be larger at depth, where θ diverges from T , where densities are greater than average surface values, and where there are larger absolute differences between pressure and depth. One may also question use of the constant density approximation in waters affected by excess evaporation (e.g., in the equatorial Pacific, Arabian Sea, and Mediterranean Sea) or large freshwater input (e.g., in the Arctic and coastal zones with heavy river influence).

To fill these gaps, we provide here an improved set of routines to model the ocean carbonate system (mocsy). This new package uses the classic approach, taking simulated A_T and C_T and computing all other carbonate system variables, while adding refinements. Relative to its precursor (OCMIP model code), mocsy offers several ameliorations: (1) it no longer makes the three approximations mentioned above, (2) it computes all carbonate system variables, not only $p\text{CO}_2$ and pH, (3) it provides these variables at all model levels, not only at the surface, and (4) it uses, as a default, the constants and the pH scale recommended by for best practices (Dickson et al., 2007). The latter are corrected for pressure effects (Millero, 1995) with modified coefficients adopted from CO2SYS (Lewis and Wallace, 1998). Options are also provided to replace formulations for K_1 and K_2 and for total boron that are recommended for best practices (Dickson et al., 2007) with more recent formulations, choices that substantially alter computed results.

After describing the mocsy code and its use (Sect. 2), we compare its results to CO2SYS, a standard software package used widely by observationalists, and evaluate how mocsy's refinements alter computed carbonate system variables (Sect. 3).

2 Methods

2.1 Basic code description

The mocsy package allows users to compute carbonate system variables from only one input pair, C_T and A_T . Those are the only two carbonate system variables that are carried as passive tracers by all ocean carbon models. Other required input variables for these calculations include temperature, salinity, PO_4^{3-} , and SiO_2 as well as pressure or depth. A precursor to mocsy was developed in 2004 and used to project future ocean acidification from simulated C_T and A_T in the OCMIP2 models (Orr et al., 2005). That precursor code was never released publicly and should not be confused with the OCMIP2 or OCMIP3 code, which only computes surface pCO_2 . Its development began by combining the Fortran code for equilibrium constants from OCMIP2 and the efficient iterative algorithm to solve for pH (Maier-Reimer, 1993; Aumont and Bopp, 2006). The precursor code was already modified to compute all carbonate system variables throughout the water column. Thus it included pressure corrections for equilibrium constants (Millero, 1995) with pressure-correction coefficients taken from version 0.95 of seacarb (Proye and Gattuso, 2003; Lavigne and Gattuso, 2011), which itself adopted code from csys (Zeebe and Wolf-Gladrow, 2001). From the seacarb code, we also included the analytical formula for the Revelle factor from Frankignoulle (1994). Our feedback from this early development led to bug corrections that were implemented in seacarb.

Since 2005, this precursor code has continued to be improved. The current release, the first public version, is denoted as mocsy. The equilibrium constants and the pH scale in mocsy are those recommended by the Guide to Best Practices for Ocean CO_2 Measurements (Dickson et al., 2007). All but three of the equilibrium constants are on the total pH scale. The first, K_S , must be referenced on the free pH scale, because it is used to convert between free and total scales. The other two exceptions are the apparent solubility products for aragonite K_A and calcite K_C (Mucci, 1983), which by definition are independent of the pH scale.

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The other basic features of mocsy also adopt the recommendations of Dickson et al. (2007). These include (1) the Weiss (1974) formulation describing the solubility of CO_2 in seawater (K_0); (2) the Lueker et al. (2000) formulations for first and second dissociation constants of carbonic acid (K_1 and K_2), refits of measurements from Mehrbach et al. (1973) on the NBS scale to the total pH scale; (3) the Millero (1995) formulations for equilibrium constants of boric acid (K_B), phosphoric acid (K_{1P} , K_{2P} , K_{3P}), silicic acid (K_{Si}), and water (K_W), converted from the seawater scale to the total scale (Dickson et al., 2007); (4) the Dickson (1990) formulation for the equilibrium constant for the dissociation of bisulfate (K_S) on the free scale (see above); (5) the Perez and Fraga (1987) formulation for the equilibrium constant for hydrogen fluoride (K_F) on the total scale; and (6) the Mucci (1983) formulations for the CaCO_3 solubility products for aragonite and calcite (K_A and K_C). Because these equilibria use concentrations instead of activities, they are apparent equilibrium constants. They are further adjusted for pressure using the approach of Millero (1995), with corrected coefficients from Lewis and Wallace (1998) (see Orr et al., 2014, Table 7). Constant ratios relative to salinity are used to compute concentrations of total boron (Uppström, 1974), sulfur (Morris and Riley, 1966), and calcium (Riley and Tongudai, 1967). The product of the Ca^{2+} and CO_3^{2-} concentrations divided by the apparent solubility product (either K_A or K_C) yields the saturation state (i.e., for aragonite Ω_A or for calcite Ω_C , respectively).

2.2 Options

Since the publication of the last best practices guide (Dickson et al., 2007), there have been developments that merit close attention given their potential impacts on computed carbonate chemistry variables. First, Lee et al. (2010) estimate that the total borate concentration in the ocean, i.e., its linear relationship with salinity, is 4 % greater than estimated previously (Uppström, 1974). Lee et al. (2010) used a more precise measurement technique on more samples ($n = 139$) collected from a wider geographic distribution than did Uppström (1974) whose total boron : salinity ratio is based on 20 samples from the deep Pacific.

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Second for K_1 and K_2 , Millero (2010) combined the same set of measurements used by Lueker et al. (2000) from Mehrbach et al. (1973) along with his own (Millero et al., 2006) to fit new formulations that are applicable over larger ranges of salinity (1 to 50) and temperature (0 to 50 °C) than are the recommended formulations of K_1 and K_2 (Lueker et al., 2000). The latter are intended to be used only when $19 < S < 43$ and $2 < T < 35$ °C. Salinities and temperatures below these thresholds do occur even in coarse-resolution global models in areas such as the Arctic, which routinely experiences subzero temperatures and intense freshwater input from rivers, land- and sea-ice melt. Generally low salinities near rivers are also common in regional models and will become more prevalent in global models as resolution increases. To model such conditions properly, we need to go beyond the best-practices recommendation (Dickson et al., 2007). Thus in mocsy, we have implemented options for the user to choose to replace the formulations for K_1 , K_2 , and total boron recommended by the best practices guide with the more recent formulations mentioned above. Likewise, for K_F we allow the user to choose either the Dickson and Riley (1979) formulation recommended by Dickson and Goyet (1994) or the Perez and Fraga (1987) formulation recommended by Dickson et al. (2007), but which is intended to be limited to waters where $10 < S < 40$ (practical salinity scale) and $9 < T < 33$ °C.

2.3 Exceptions to best practices

The best-practice formulations for K_W , K_{1P} , K_{2P} , and K_{3P} proposed by Dickson et al. (2007) are those from Millero (1995) with 0.015 subtracted from the constant term as a simple means to convert from the seawater to the total hydrogen ion scale (Dickson and Goyet, 1994; Dickson et al., 2007, Chap. 5, footnote 5). In mocsy, we do not impose this constant correction, preferring instead to use the classic approach to convert equilibrium constants between the two pH scales (e.g., Millero, 2010, Eq. 6), resulting in a pH-scale correction that varies with [HF]. The same variable correction is used in CO2SYS.

Dickson et al. (2007) do not discuss pressure corrections of equilibrium constants. For that, mocsy follows the lead of CO2SYS using Millero's equations, quadratic functions of pressure and temperature (Millero, 1995, Eqs. 90–92) with corrections to associated coefficients from Lewis and Wallace (1998) as detailed in a recent comparison (Orr et al., 2014, Table 7).

2.4 Evaluation

To validate mocsy, its computed variables were compared to those from CO2SYS-MATLAB (van Heuven et al., 2011) run with identical input data. Input data for A_T and C_T are from the three-dimensional, global gridded data product on a $1^\circ \times 1^\circ$ grid known as GLODAP (Key et al., 2004). The other input data are taken from the 2009 World Ocean Atlas gridded data product, which includes in situ temperature (Locarnini et al., 2010) and salinity (Antonov et al., 2010) as well as phosphate and silicate concentrations (Garcia et al., 2010). The CO2SYS code was chosen as the reference because it was the first publicly available software package (Lewis and Wallace, 1998) and it may still be the most widely used by the community. Furthermore, it has been updated regularly, and a close inspection of the code and documentation reveals the extreme care that has gone into its development and the process of rooting out potential errors.

3 Results

3.1 Evaluation

Our evaluation reveals that mocsy's computed variables differ from those computed with the CO2SYS-MATLAB package, but generally by less than 0.005%. Consistently small differences are found for area-weighted, global average vertical profiles (Fig. 1) as well as for surface zonal means (Fig. 2) of computed $p\text{CO}_2$ and concentrations of CO_3^{2-} , HCO_3^- , CO_2^* , and H^+ . Disagreement is larger yet remains small for computed Ω_C

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(up to 0.07%) and Ω_A (up to 0.13%) The largest disagreement is found for mocsy's computed Revelle factor, which reaches up to 0.7% greater in Southern Ocean surface waters and up to 1.5% larger at 5000 m, on average.

3.2 Model approximations

5 The three approximations that have been widely used in models lead to significant errors in some computed variables in the deep ocean (Fig. 3). For $p\text{CO}_2$, the total error is $-1\ \mu\text{atm}$ at 1000 m and $-8\ \mu\text{atm}$ at 5000 m, almost entirely from the temperature approximation. There is only a slight compensation by the error from the pressure approximation (e.g., reaching $+0.5\ \mu\text{atm}$ at 5000 m). The constant density approximation
10 produces no significant error neither for $p\text{CO}_2$ nor for any of the other computed tracers. For pH, the total error also grows with depth reaching up to $+0.010$ at 5000 m. Most of that derives from the temperature approximation, but the pressure approximation also contributes in the same direction. For CO_3^{2-} , the total error remains negligible, with small errors from the temperature approximation (e.g., $-0.2\ \mu\text{mol kg}^{-1}$ at 5000 m)
15 being compensated by nearly equal and opposite errors from the pressure approximation. Errors in Ω_A have a similar pattern but the error from the pressure approximation weighs more heavily leading to a slight total error of $+0.01$ units at 5000 m. The difference in relative errors between Ω_A and CO_3^{2-} is thus due to the dominance of the error from the pressure induced variability in the K_A outweighing the sensitivity to temperature. For computed CO_2^* and the Revelle factor, the errors are similarly dominated
20 by the temperature approximation and grow with depth but even at 5000 m they reach only $-0.005\ \mu\text{mol kg}^{-1}$ and -0.01 units, respectively.

3.3 Options

25 The effects of the three options on computed variables differ by region and depth. The choice for the K_F option has little effect on computed quantities and can be neglected.

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Conversely, there are substantial differences that depend on the choice of the two other new options: total boron and the formulations for K_1 and K_2 .

The new formulation for total boron (Lee et al., 2010) increases borate alkalinity A_B by about 4%. Yet modeled total alkalinity A_T is unaffected, being an input variable (along with C_T). Since A_T is unchanged and A_B is higher, then modeled carbonate alkalinity A_C must be lower. This decline in A_C reduces surface CO_3^{2-} everywhere, from $-1.5 \mu\text{mol kg}^{-1}$ in the Southern Ocean to $-3 \mu\text{mol kg}^{-1}$ in the tropics (Fig. 4). The corresponding decline in surface Ω_A is between 0.02 to 0.04. Simultaneously, computed surface $p\text{CO}_2$ increases by 4 to $6 \mu\text{atm}$ and surface pH declines by 0.006 units. Nonetheless the Revelle factor declines by 0.04, i.e., the buffer capacity increases. That is, despite the reduced CO_3^{2-} and increased $p\text{CO}_2$, by maintaining the same total alkalinity while reducing carbonate alkalinity, the C_T must also decline. Hence the A_T minus C_T increases, as must then the buffer capacity. In the deep ocean, the new total boron formulation leads to nearly uniform changes in $p\text{CO}_2$ of $+5 \pm 1 \mu\text{atm}$, in pH of -0.005 ± 0.001 units, and in CO_3^{2-} of $-1 \pm 0.1 \mu\text{mol kg}^{-1}$ (Fig. 5).

4 Discussion

The constant density approximation imposes that the same density, typically 1028 kg m^{-3} , be used to convert input (A_T , C_T , and nutrients) from model concentration units (mol m^{-3}) to data units (mol kg^{-1}) as needed for the equilibrium calculations. Resulting concentrations of computed variables (e.g., CO_3^{2-}) are then reconverted back to model units with the same density. When the same constant density is used in all subsequent analysis that compares computed variable concentrations to data (converting from mol m^{-3} to $\mu\text{mol kg}^{-1}$ or vice-versa), errors are always negligible. Conversely, if a different constant density or a variable density is used in subsequent model-data comparison, associated errors can surpass those from the other two

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approximations. Hence mocsy avoids the constant density approximation, while also providing the model's in situ density as output.

So far, we have focused on quantifying errors in computed variables from the three model approximations and in assessing how variables are affected by the three user options. A more general concern is how computed variables are affected by the frequent practice of neglecting nutrient concentrations in carbonate system calculations. In high-nutrient regions, the changes in computed variables due to phosphate and silicate alkalinity (Figs. 6 and 7) are similar in magnitude and have the same sign as those due to the change to the new formulation for borate alkalinity (Figs. 4 and 5). All three contribute to non-carbonate alkalinity and hence total alkalinity,

$$A_T = A_C + A_B + A_W + A_P + A_{Si} + A_O, \quad (1)$$

where

$$A_C = [\text{HCO}_3^-] + 2 [\text{CO}_3^{2-}], \quad (2)$$

$$A_B = [\text{B(OH)}_4^-], \quad (3)$$

$$A_W = [\text{OH}^-] - [\text{H}^+]_F, \quad (4)$$

$$A_P = [\text{HPO}_4^{2-}] + 2 [\text{PO}_4^{3-}] - [\text{H}_3\text{PO}_4], \quad (5)$$

$$A_{Si} = [\text{SiO(OH)}_3^-], \text{ and} \quad (6)$$

$$A_O = [\text{NH}_3] + [\text{HS}^-] - [\text{HSO}_4^-] - [\text{HF}] + \dots \quad (7)$$

In words, the contributions on the right side of Eq. (1) come from components of carbonic acid, boric acid, water, phosphoric acid, silicic acid, and other species, respectively. The latter include bisulfate (also used to convert between free and total pH scales) and hydrogen fluoride (used to convert between total and seawater scales). As an input variable, A_T is not affected by the choices such as using a more simplified alkalinity equation, neglecting nutrient concentrations, or choosing a different formulation for total boron. Yet A_C is affected, being computed by difference. As any of A_B , A_P ,

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or A_{Si} increase, computed A_C must decrease. In the surface ocean, nutrient alkalinity ($A_P + A_{Si}$) substantially alters computed carbonate system variables where nutrient concentrations are largest, e.g., in the equatorial Pacific and in the high latitudes (poleward of 40°). The largest surface effects occur in the Southern Ocean where computed pCO_2 changes by $+6 \mu\text{atm}$, once nutrients are accounted for, which is six times more than estimated by Follows et al. (2006). At the same time, CO_3^{2-} changes by $-1.6 \mu\text{mol kg}^{-1}$ and pH by -0.007 (Fig. 6).

These biases concern models that carry only practical alkalinity ($A_C + A_B + A_W$), i.e., which neglect alkalinity from phosphoric and silicic acids. Equivalent biases occur when nutrient concentrations are assumed to be zero in offline calculations with output from models that include these nutrients in the alkalinity equation. Without other compensating biases, this simplification would lead to a simulated aragonite saturation horizon that is too deep (Fig. 8), a simulated onset of aragonite undersaturation in polar surface waters ($\Omega_A < 1$) that is too late, and a simulated interhemispheric north-to-south oceanic transport of carbon (Sarmiento et al., 2000) that is too weak. Our results illustrate where and by how much models err when they neglect nutrient alkalinity, either because of a simplified alkalinity equation or equivalently by assuming null nutrient concentrations (e.g., in offline calculations). Remedying these errors requires little extra coding and does not add significantly to a model's computation time. For models that do not carry PO_4^{3-} and SiO_2 as tracers, the bias in computed carbonate system variables would be reduced by imposing that alkalinity from those absent tracers follow observed nutrient climatologies (Garcia et al., 2010).

When combined with the new formulation for total boron (Lee et al., 2010), the magnitude of the total change in the deep ocean is nearly double that from nutrients alone (sum from Figs. 4 and 6). On average, the combined effect in the deep ocean shifts CO_3^{2-} by $-3 \mu\text{mol kg}^{-1}$, pH by -0.018 , and pCO_2 by $18 \mu\text{atm}$ (sum from Figs. 5 and 7). The combined effect also shallows the computed modern ASH by about 100 m in the North Atlantic and up to 300 m in the Southern Ocean (Fig. 8).

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5 Conclusions

For simplicity, modelers typically make ocean carbonate chemistry calculations with the following three assumptions: (1) that model density is constant, (2) that simulated potential temperature is an adequate proxy for in situ temperature, and (3) that model depth is equivalent to pressure. None of the three approximations produces significant errors at the surface. Below the surface, errors in some variables grow with depth due to combined effects from the temperature and pressure approximations; the constant density approximation does not contribute unless a different density is used to convert computed concentrations, e.g., to $\mu\text{mol kg}^{-1}$. At 5000 m, total errors from the temperature and pressure approximations reach $8 \mu\text{atm}$ in $p\text{CO}_2$, $+0.010$ in pH, $+0.1 \mu\text{mol kg}^{-1}$ in CO_3^{2-} , and $+0.005$ in Ω_A . The mocsy modeling routines avoid these errors with little additional coding and trivial increases in computational time.

The same code also offers two new options to provide for developments since the publication of the best practices guide (Dickson et al., 2007). Those options concern an assessment that seawater contains 4% more total boron than thought previously (Lee et al., 2010) and new formulations for K_1 and K_2 designed to include low salinity waters (Millero, 2010). The new boron option leads to substantial shifts in computed surface variables, e.g., $+4$ to $+6 \mu\text{atm}$ in $p\text{CO}_2$, -1.2 to $-2.5 \mu\text{mol kg}^{-1}$ in CO_3^{2-} , and -0.006 in pH. Comparable shifts at depth lead to a shallower computed ASH by 50 m in the North Atlantic and by up to 90 m in the Southern Ocean. The new option for K_1 and K_2 leads to an even larger shift of $+7 \mu\text{atm}$ in surface $p\text{CO}_2$ in the Southern Ocean. When both options are combined, the Southern Ocean's surface $p\text{CO}_2$ becomes $3 \mu\text{atm}$ higher than in the high northern latitudes and $6 \mu\text{atm}$ higher than in the tropics. A third option, specifying use of the Dickson and Riley (1979) formulation for K_F instead of that recommended for best practices (Perez and Fraga, 1987) produces no significant differences.

Of additional concern is the common modeling practice of neglecting nutrients, either in the model's equation for alkalinity (practical alkalinity) or the equivalent assumption

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that nutrient concentrations are zero. Resulting errors in computed surface $p\text{CO}_2$ have similar magnitudes and patterns as do the shifts associated with the change in the formulations for K_1 and K_2 . They too lead to similar meridional differences in surface $p\text{CO}_2$. Accounting for nutrient alkalinity further shallows the computed ASH, e.g., by about 50 m in the North Atlantic and by 100 to 200 m in the Southern Ocean.

Therefore, modelers would do well to avoid the three common approximations, to use the new boron option, and to account for nutrient alkalinity in model equations and offline calculations. Although, the new formulations for K_1 and K_2 also lead to large differences in computed variables, we consider their use premature, because the published sets of coefficients have an inadequate number of significant figures and are inconsistent among the different pH scales (Orr et al., 2014). As open software, modelers are free to use mocsy directly or borrow from it to refine their simulated carbonate chemistry and air–sea CO_2 fluxes.

Code availability

The mocsy package is distributed under the MIT license and is available from github. It can be retrieved in the conventional manner with git, namely by issuing the following command

```
git clone git://github.com/jamesorr/mocsy.git
```

in an X terminal on Linux, Mac or PC operating systems. If that fails, install git and try again, or go to the main web page on github <https://github.com/jamesorr/mocsy> and click on the link “Download ZIP”. Once downloaded, mocsy can be compiled by typing

```
make
```

More details on the code, its compilation, and examples of its use in Fortran and when called from python can be found in the mocsy manual at <http://ocmip5.ipsl.jussieu.fr/mocsy/>.

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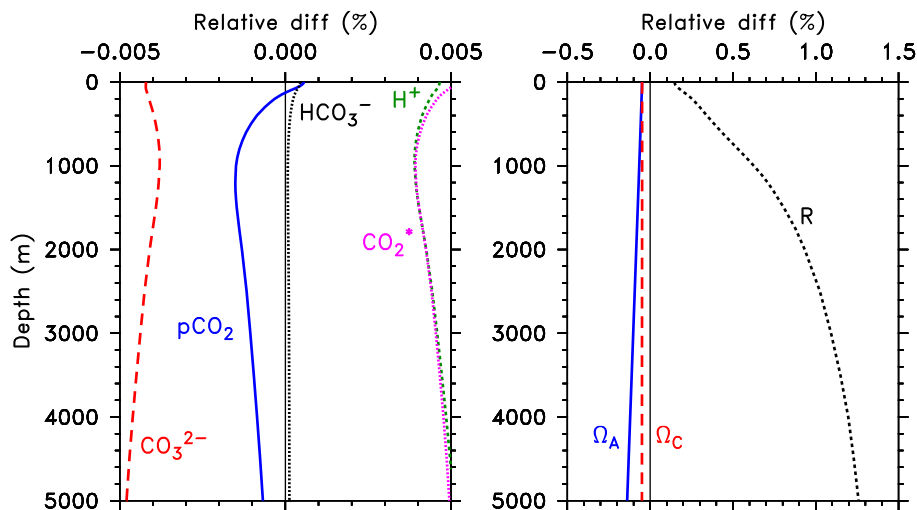
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Fig. 1. Global-mean vertical profiles for the relative difference between mocsy and CO₂SYS for each computed variable $100(V_{\text{mocsy}} - V_{\text{co2sys}})/V_{\text{co2sys}}$.

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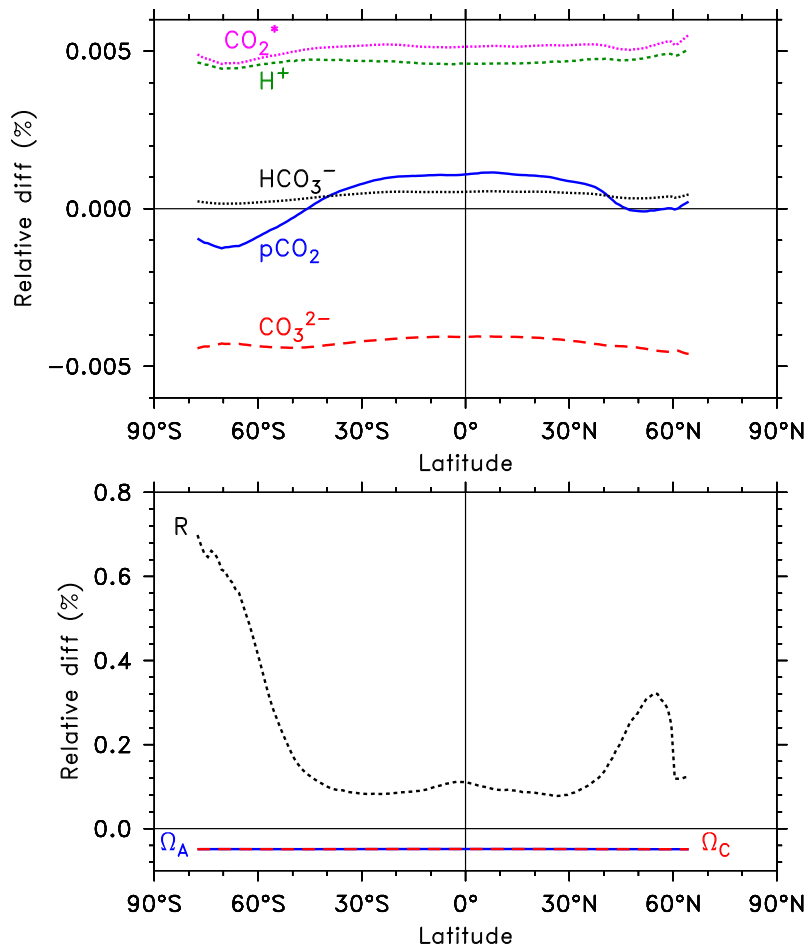
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Fig. 2. Surface zonal mean of the relative difference for computed variables, computed as in Fig. 1.

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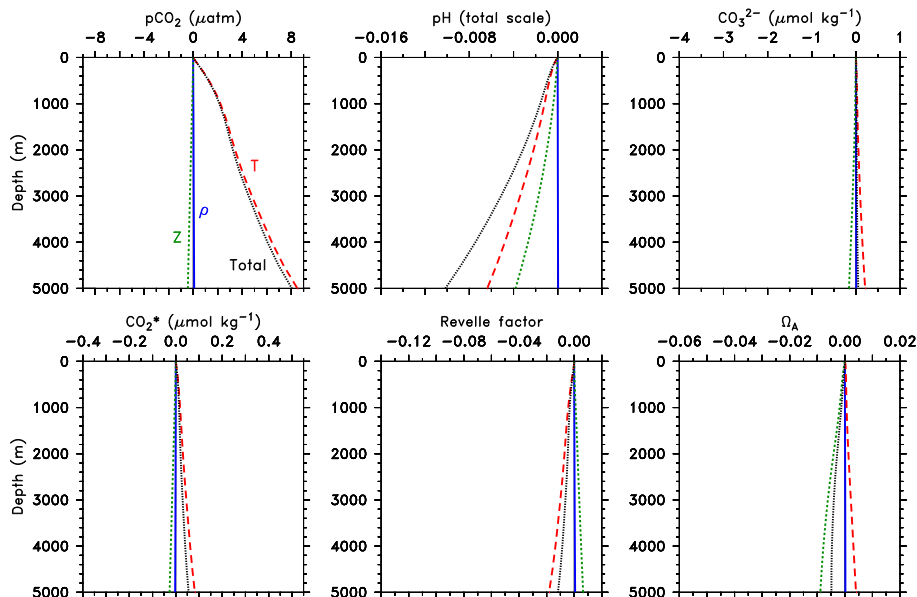


Fig. 3. Global-mean vertical profiles of corrections that need to be applied for each of the three ocean-model approximations: (1) that density is constant (blue ρ), (2) that potential temperature is equivalent to in situ temperature (red T), and (3) that depth (m) is equivalent to pressure (dbar) (green Z). Associated errors are equal but opposite in sign to each correction.

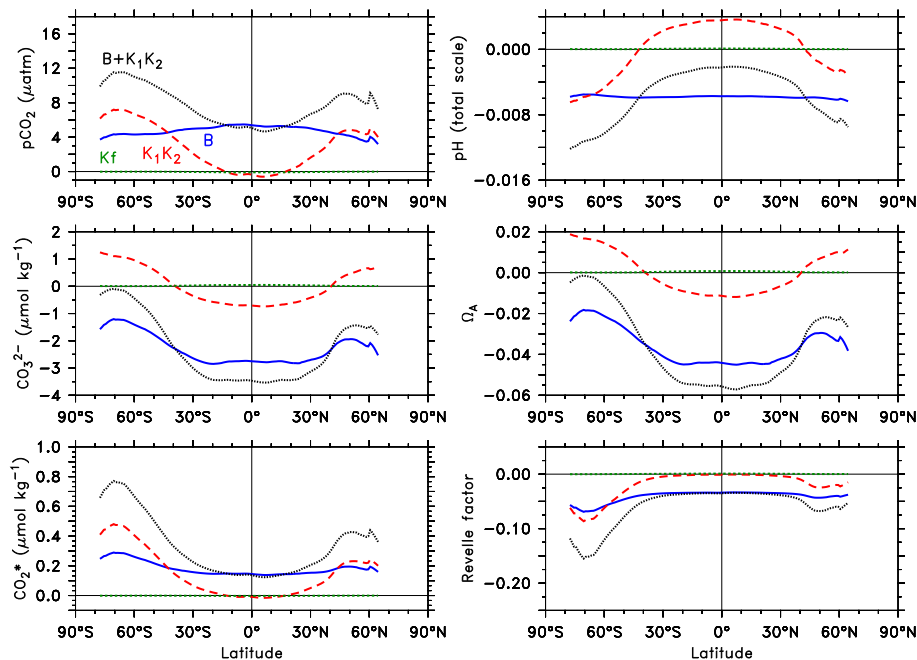
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Fig. 4. Zonal mean of changes in computed variables after replacing best-practice recommendations with two newer options: (1) the Lee et al. (2010) formulation for the total boron-to-salinity ratio (blue B), (2) the Millero (2010) formulations for K_1 and K_2 (red, K_1K_2). Differences are shown relative to (1) Lee et al. (2010) and (2) Lueker et al. (2000).

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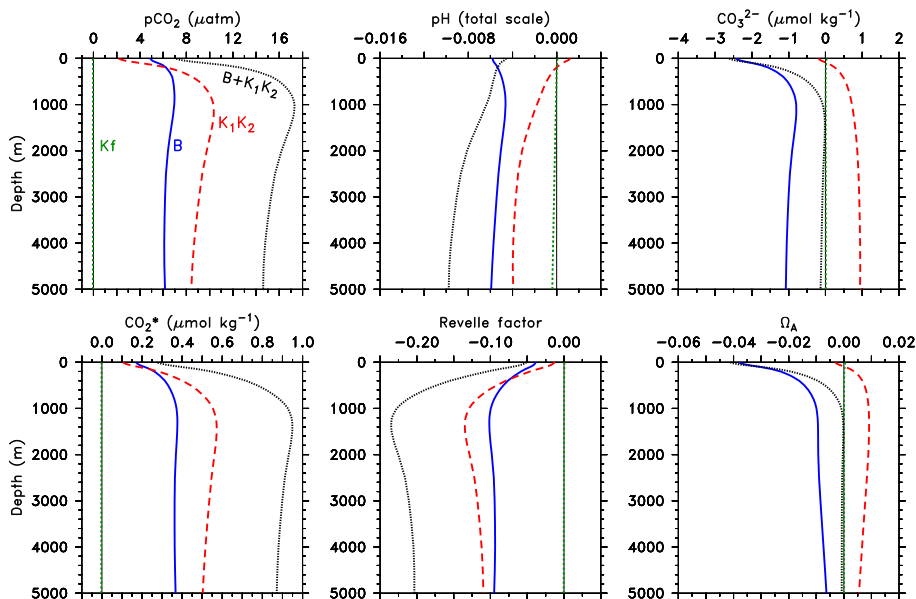


Fig. 5. Changes in global-mean vertical profiles of computed variables after replacing best-practice recommendations with the same two options as detailed in Fig. 4.

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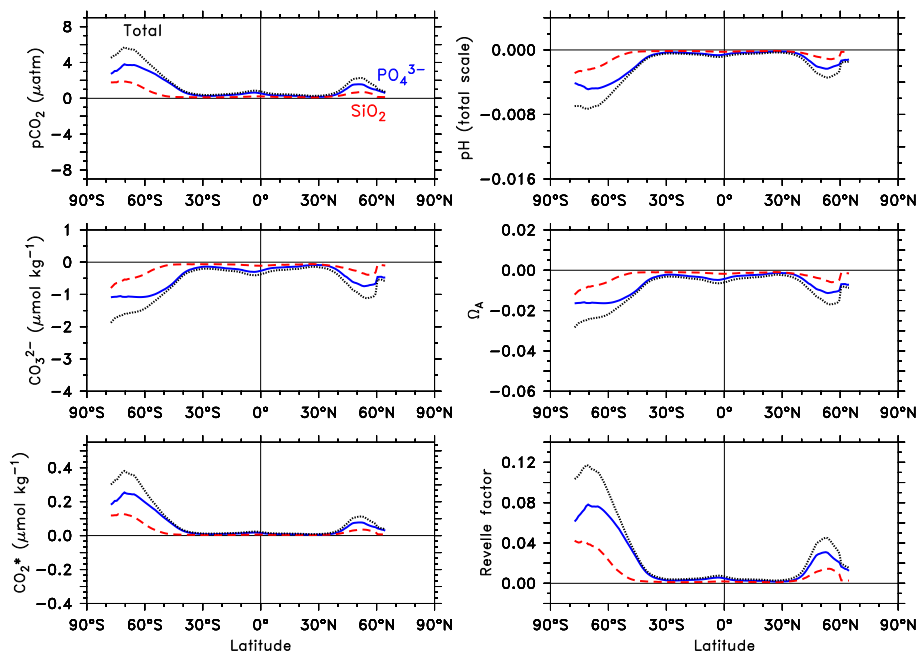


Fig. 6. Zonal mean changes in computed variables due to alkalinity contributions from phosphate (blue solid), silicate (red dashed), and their sum (black dotted) relative to the case where nutrient alkalinity is neglected (practical alkalinity).

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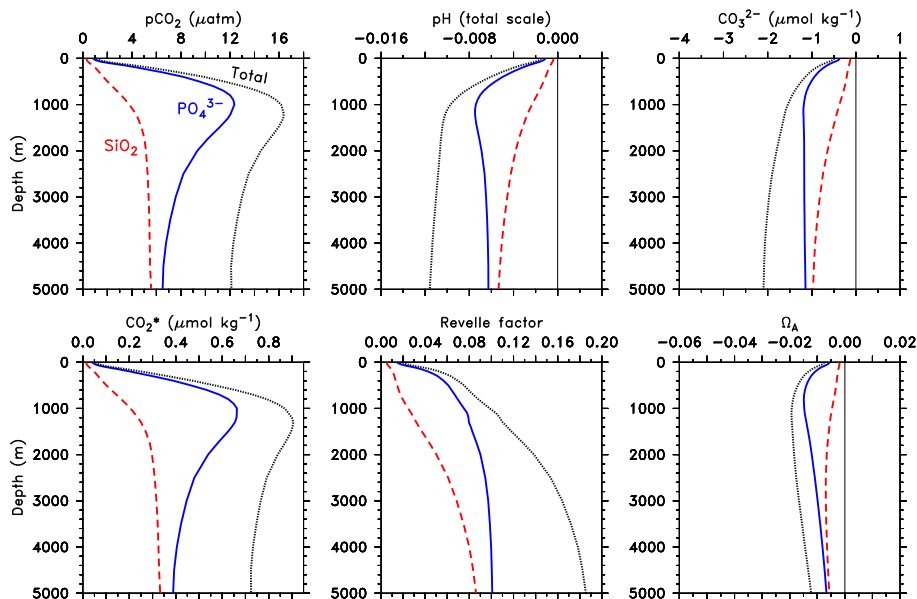


Fig. 7. Global-mean profiles of the changes in computed variables attributable to nutrient alkalinity, i.e., for the same components shown in Fig. 6.

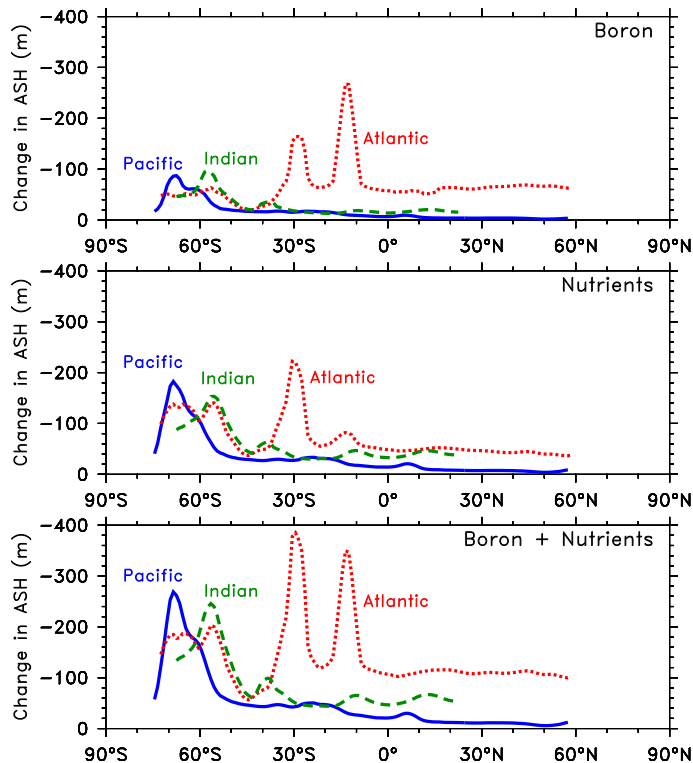


Fig. 8. Changes in the aragonite saturation horizon (ASH) due to (top) using the new formulation of total boron (Lee et al. minus Uppström), (middle) accounting for nutrient alkalinity (total minus practical alkalinity), and (bottom) summing both corrections. Changes in ASH (m) are smoothed over 5° bands of latitude and shown for zonal means over the Atlantic, Pacific, and Indian Oceans. The peaks at 30° S and 12° S in the Atlantic are caused by subtle shifts in horizontal gradients of Ω_A .

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