A fast parameterization of carbonate burial and dissolution for the earth science box modeling toolkit (ESBMTK)

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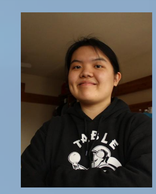
Tina Tsan


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Objective

The Earth Sciences Box Modelling Toolkit (ESBMTK) provides several python classes (e.g., Air-Sea gas exchange, seawater chemistry, hypsometry, etc.) which simplify typical box-modelling tasks in the earth sciences.

We aim to extend the ESBMTK framework with modules which describe processes relevant to marine carbonate chemistry. This includes functions to calculate carbon speciation in seawater, as well as computationally efficient parameterizations for carbonate burial and dissolution.

Carbonate Chemistry

If the rates of CO_2 solution/outgassing, organic matter production, and carbonate precipitation are known, ESBMTK can model the concentrations of the conservative seawater properties of dissolved organic carbon (DIC) and total alkalinity (TA).

However, carbonate dissolution (and possibly carbonate precipitation) depends on and affects the carbonate ion concentration. In the first step, we calculate the various dissolved carbon species,

$$DIC = [CO_2]_{aq}^* + [HCO_3^-] + [CO_3^{2-}]$$

$$TA = [HCO_3^-] + 2[CO_3^{2-}] + \text{minor species}$$

using the iterative approach of Follows et al. (2006). The carbonate ion concentration is then used to calculate the following depth intervals using the equations of Boudreau et al. (2010) (see equations in Fig. 2).

- zsat: The depth where the $CaCO_3 \leftrightarrow Ca^{2+} + HCO_3^-$ is in equilibrium
- zcc: The depth where the rate of $CaCO_3$ dissolution is equal to the export flux of $CaCO_3$
- zsnow: The depth where sediments become carbonate-free

Once these depths are known, we use the parameterizations of Boudreau et al. (2010) to calculate the respective burial/dissolution fluxes (see equations in Fig. 2) and update the concentrations of TA and DIC accordingly.

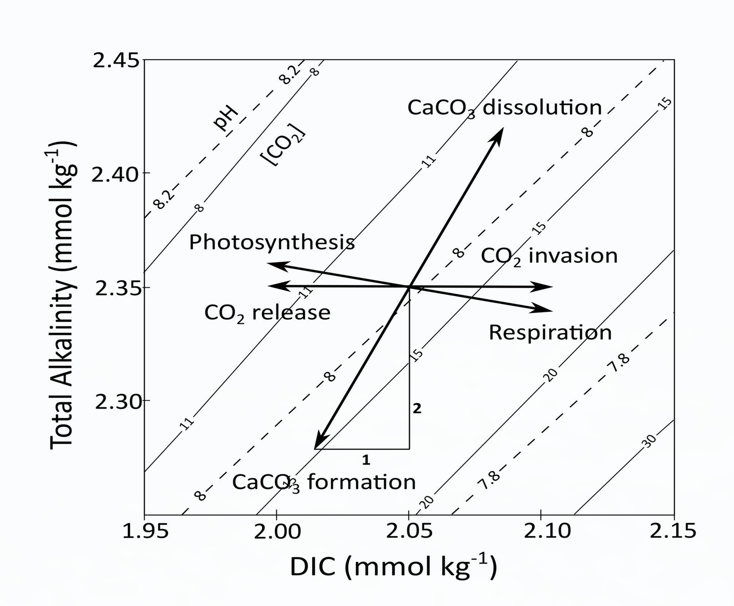

Figure 1. Figure from Zeebe & Wolf-Gladrow (2001). The arrows indicate how DIC and TA are affected by different processes. Constant levels of dissolved CO_2 in µmol kg^{-1} and pH are indicated by the solid and dashed lines, respectively. As an example, $CaCO_3$ formation reduced DIC by 1 mmol kg^{-1} and TA by 2 mmol kg^{-1}. As a result, this increases CO_2 levels but decreases the pH within the system.

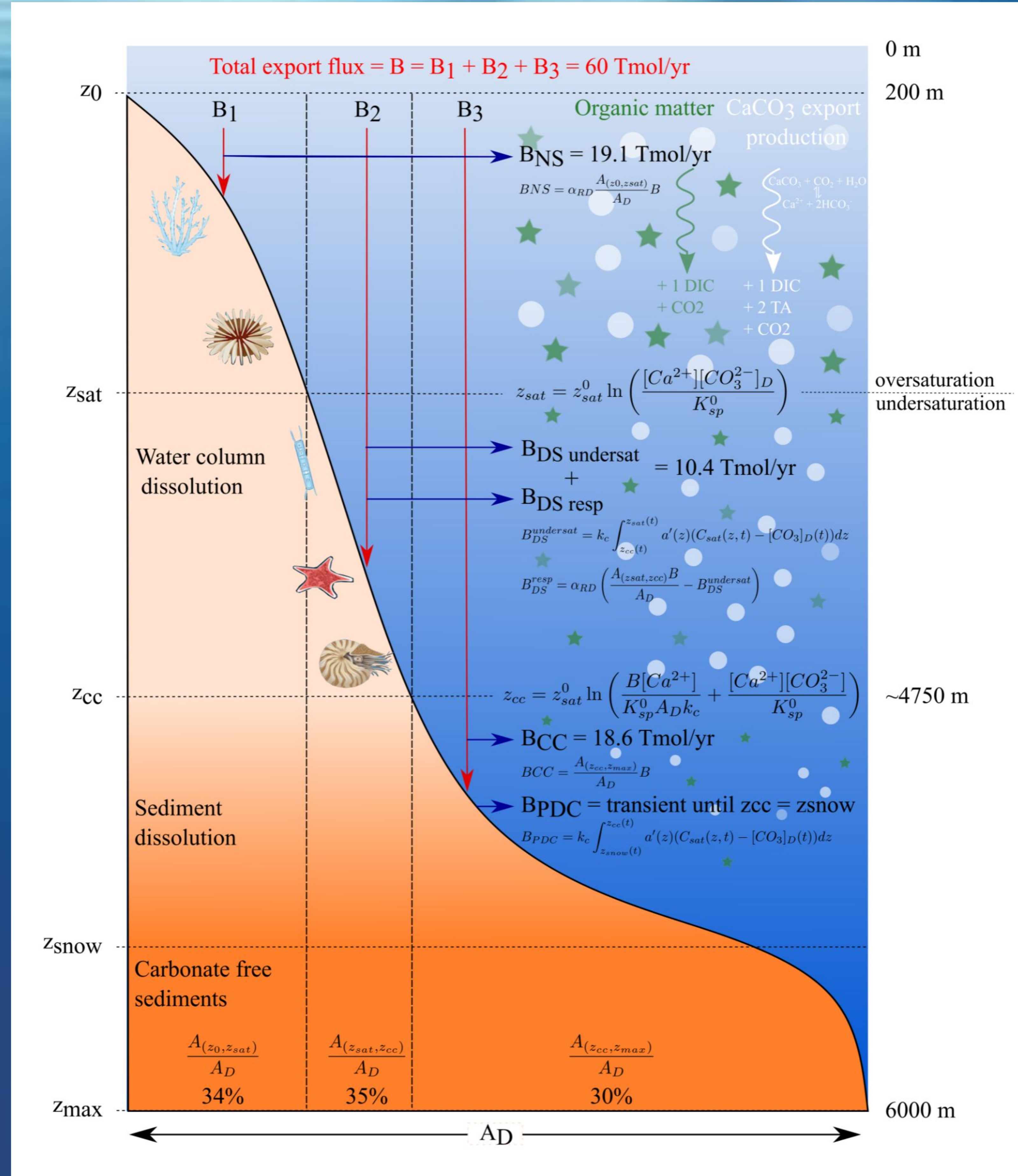

Figure 2. Diagram showing ocean schematic with horizon depths and calcite flux movements for the deep box.

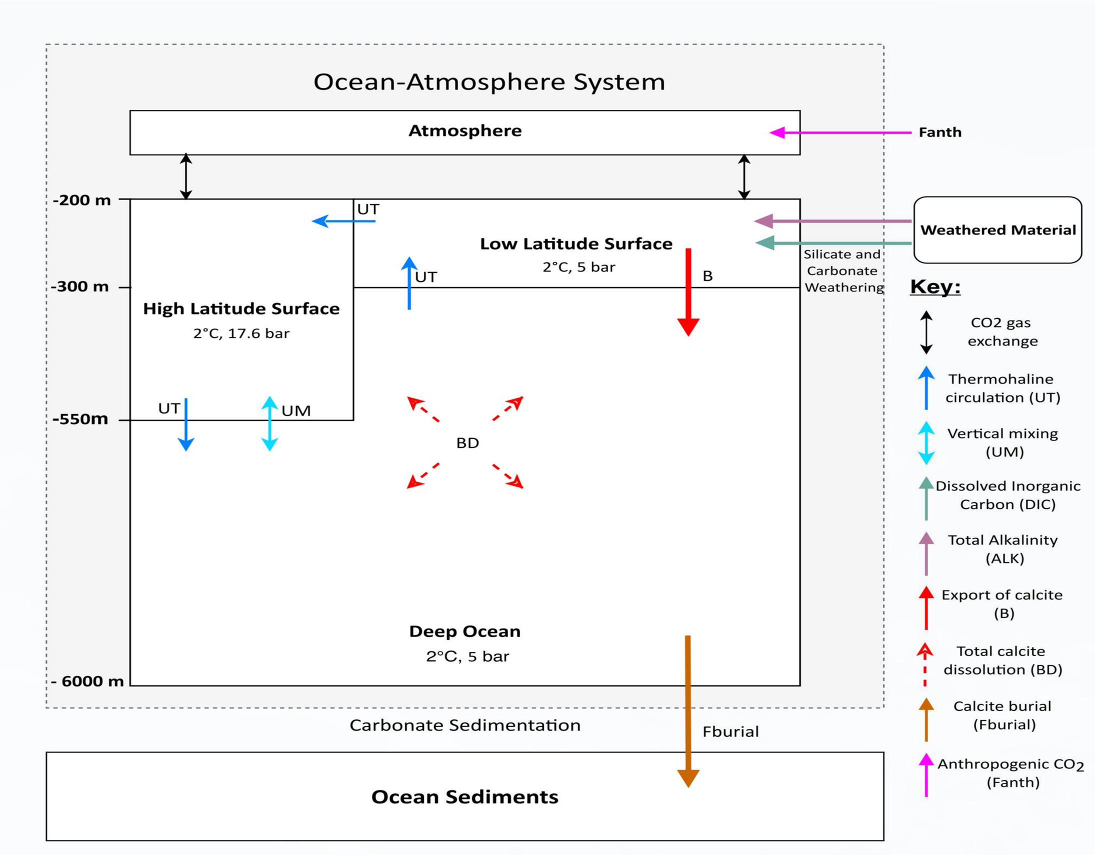

Figure 3. The 4-box model for the carbonate system of the oceans in ESBMTK and the associated flux movements. The ocean is divided into 4 boxes for low latitude surface, high latitude surface, deep ocean and the atmosphere.

Benchmarking

Boudreau et al. (2010) use a modified Harvardton-Bear 3-box model (Sarmiento & Toggweiler, 1984). Here we re-implement their model using the ESBMTK framework, and then add our new classes to test the implementation of our new classes against their results.

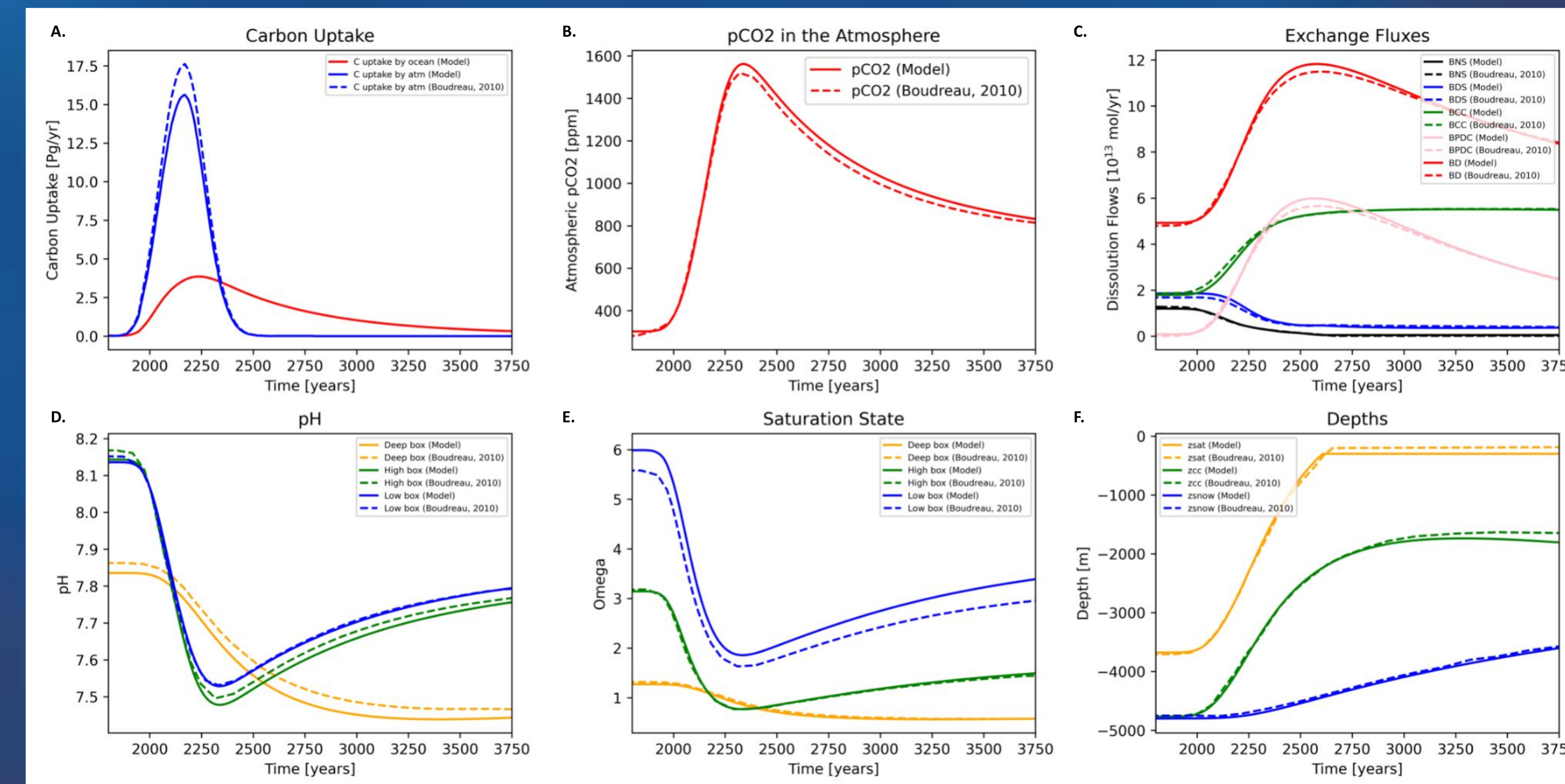

Figure 4. Comparison between the ESBMTK model results and digitized model results from Boudreau et al. (2010). **(a)** Carbon uptake by the ocean and atmosphere **(b)** Partial pressure of CO2 in the atmosphere **(c)** Dissolution fluxes within the deep box (See Fig. 2) **(d)** pH **(e)** Saturation state **(f)** Positions of the critical horizons in the deep box: *zsat*, calcite saturation horizon; *zcc*, carbonate compensation depth; *zsnow*, snowline

Discussion

One of the major challenges faced was matching model output values with the results in Boudreau et al. (2010). Fortunately, we were able to access the original model code provided by Boudreau et al. (2010) which helped with debugging and fine-tuning model parameters, allowing us to attain reasonable results (See Fig. 4).

Another challenge was the extension of the framework itself which required new functions and also editing of pre-existing functions within multiple classes of ESBMTK. Consistent communication via Google Meets and Discord, as well as Git enabled us to effectively collaborate on the code together simultaneously. Debugging new code also required tedious amounts of testing but major bugs were resolved by reducing the complexity and isolating the code.

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We would like to thank Professor Wortmann for his guidance throughout the project. Additional thanks to the Centre for Global Change Science (CGCS) at the University of Toronto and the Natural Sciences and Engineering Research Council of Canada (NSERC) for supporting this project. Special thanks to Bernard Boudreau and Filip Meysman for providing us with the source code for the box model in Boudreau et al. (2010).

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