Interactive comment on "Implementation and assessment of a carbonate system model (Eco3M-CarbOxv1.1) in a highly-dynamic Mediterranean coastal site (Bay of Marseille, France)" by Katixa Lajaunie-Salla et al.

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1 General comments

1.1 Appreciation of the manuscript

In this paper, K. Lajaunie-Salla and co-authors present Eco3M-CarbOx, a biogeochemical model of the carbonate system and the plankton food web. It is integrated into the Ecological, Mechanistic and Modular Modelling framework, Eco3M (Baklouti et al., 2006b). In the paper, it is applied to the Bay of Marseille (Mediterranean Sea) for which there are comprehensive data time series available. I found the study interesting, but the paper has, unfortunately, a number of weaknesses. The paper is well-readable, but there remain numerous English errors. This manuscript has been submitted as a "model description paper." The model description in the main text reduces to thirty-two lines of text only (plus a schematic and a few equations in the appendix), of which fifteen deal with the new carbonate system module. These fifteen lines contain only a few commonplace statements followed by a sequence of eleven reference citations. This is far from what I expect to read in a "model description paper" in Geoscientific Model Development. It is also far from what is expected for that type of publication (see http://www.geoscientific-model-development.net/about/manuscript_types.html#item1). Accordingly, I do not even think that this manuscript fits the scope of the journal in its current form. Details about the approximations, numerical methods adopted and algorithms used, their applicability and their limitations are completely missing. Furthermore, some of the model experiments also have critical shortcomings: it is not realistic to assume that river water intrusions only impact the Total Alkalinity, TA, budget but not that of Dissolved Inorganic Carbon, DIC (riverine TA is mainly carried as HCO_3 which impacts the DIC and the TA budgets alike). For upwelling events, only a temperature effect is considered. However, upwelling events also bring nutrients, DIC and TA to the surface. The effects of these latter are not considered in the paper, possible effects not even discussed. I think the authors will first have to make up their mind whether they want to consider their manuscript as a "model description paper" in Geoscientific Model Development, or whether they would prefer to focus on the data analysis and interpretation. In both cases, they will have to extend the model description and revise the experimental design; in the second case, it would be recommended to submit this paper in other journal, such as, e.g., the sister journal Biogeosciences.

I am nevertheless convinced that this paper could make a valuable contribution to Geoscientific Model Development: from what I have been able to grasp from the paper and the code, the model approach looks solid and it could certainly be applied to other regions of the World as well. I therefore encourage the authors to go for the first option and prepare a **major revision** of their manuscript that includes a comprehensive model description and a sound experimental design.

Reply: We thank the reviewer for the evaluation of our work to be published in GMD journal. We thank too him for the detailed and useful comments that contributed to greatly improve the manuscript. We consider his comments to improve the manuscript. We agree that is missing information about the new carbonate system module. In this way, we propose to add all the details of the carbonate system module in appendix (see the appendix is at the end of this document). Concerning the riverine inputs scenarii, we decide to focus on nitrate and alkalinity supply. In fact the model simulates the DIC increases, as is observed, which highlight that the carbonate system module is well resolved.

In this study we did not experiments the impact of an upwelling events (with a decrease of temperature). During upwelling events the seawater temperature could decrease by 5°C, which explain the strong temperature variations observed during summer (Fig.4A). Observations show strong variations of carbonates system variables during summer, which reproduce the model. These results are explained in the section 3.2 L280-285 of the MS.

2 Specific comments

2.1 Abstract

The abstract is not well focused and the hesitation between a model description and a data analysis approach is strongly visible.

Reply: Here, we think that the reviewer was confused with the windy periods, upwelling and temperature changes. Looking the temperature time series along the year 2017, we observe strong temperature variation in summer. These variations are due to upwelling events that bring bottom cold water to the surface. These upwelling events occur under specific wind direction and when the velocity is high, as during Mistral wind periods. To be clearer we modify the L24-26 as following:

"Upwelling events change seawater temperature quickly, which alter the behavior of the BoM waters within a few days from a source of CO_2 *to the atmosphere to a sink into the ocean."*

2.2 Model description

The model description is completely insufficient. For the underlying model, upon which Eco3M-CarbOx is built, only the ecological structure is summarized. Nothing is said about the spatial extension adopted: is it a point model? does it have some spatial extensions? 1D, 2D, 3D? In the code, one can see that state variable arrays are threedimensional, but it is not clear if the three spatial dimensions are actually used: the applied pressure, e.g., is set to 1 bar throughout, as if the model was applied for a water depth of about 10m only. If the model has some spatial extension, how are the lateral and bottom boundaries treated? The physical processes, although mentioned from time to time, are not at all dealt with here. How are they (e.g., transport processes) represented? This lack of description is rather incomprehensible as the authors themselves emphasize in their description of the study area that the biogeochemistry in the Bay of Marseille is "highly driven by hydrodynamics" (p. 3, l. 99).

Reply: We agree that this information was not clear in our previous version of the MS: The spatial dimension of the model is 0 in this study. The state variables of the model only change along time. As in this work the biogeochemical model is not coupled with a hydrodynamic model, the circulation is not taking into account. We add this information in L114-116, as following:

"In this study, the state variables of the Eco3M-CarbOx model only change along time (i.e. usually termed "model 0D"), are representative of the time evolution of a sea surface water cell but this biogeochemical plankton model is not coupled with a hydrodynamic model."

Any carbonate system speciation calculation procedure rests upon a TA approximation and a pH solver. Here, we do not read anything about these two elements:

- What TA approximation is adopted, i.e., which acid-base systems are taken into account?
- What pH-scale is adopted?
- Which numerical method is used to solve the resulting pH equation? What are the limitations of the adopted method (some methods fail to converge for low salinity water samples, e.g.)?
- Which parametrisations have been used for the stoichiometric constants?

I have been able to find answers to some of these questions by browsing though the code (although I am still not sure which pH scale is actually used in the end—probably pHtot). These informations must nevertheless be given in the main paper. It should not be necessary to inspect the code to find such basic informations.

As the model description stands, there is no way to reproduce the model results, a main requirement of model descriptions in Geoscientific Model Development.

Reply: We agree with the reviewer that information about the carbonates system speciation is not clearly specified. To resolve the carbonate system we use the value of DIC and TA to determine the value of pH and pCO2 and we use the total pH scale. DIC and TA are states variables of the Eco3M-CarbOx model.

The biogeochemical processes that impact DIC dynamics are: photosynthesis and respiration of phytoplankton, respiration of bacteria and zooplankton, precipitation and dissolution of CaCO3, and the CO2 exchange with the atmosphere.

The biogeochemical processes that impact TA dynamics are: uptake of nutrients by phytoplankton, mineralization of nitrogen organic matter by bacteria, nitrification and, precipitation and dissolution of CaCO3.

Taking into account the comments of the reviewer we propose to add an Appendix that gives all details about the resolution of the carbonate system. The appendix is at the end of this document. We add this following sentence L143-145:

"The details of the resolution of carbonate system module are given at the appendix B. For this module three processes were also added: the precipitation and dissolution of calcium carbonate and the gas exchange of pCO2 with the atmosphere."

2.3 Experimental design

As mentioned above, I find that there are inconsistencies in the design of the model experiments. In the model upwelling events, only a temperature effect is taken into account. However, as stated on p. 3, l. 100, such events also bring nutrient rich waters to the surface. Accordingly, they should also perturb the nitrate, DIC and TA balances. This is not what the model results reflect: they witness of cooling events only. Similarly, only part of the effects of Rhône river plume intrusions on the carbonate system are taken into account: the experiments only consider the resulting TA perturbation, but not the DIC perturbation. To my best knowledge, rivers mainly carry TA in the form of HCO_3^- which impacts the DIC balance as strongly as the TA budget. I am even wondering—but could not find any decent data—if the River Rhône water does not also have high pCO_2, in which case it would even carry more DIC than TA.

Reply: In this study we did not experiments the impact of an upwelling events (with a decrease of temperature). We evaluate the impact of different forçings: the temperature, wind, intrusion of nutrients, alkalinity, and atmospheric CO2.

In the BoM, upwelling events occurs during wind-specific conditions, as Mistral wind. During these days the seawater temperature could decrease by 5°C, which explain the strong temperature variations observed during summer (Fig.4A). Observations show strong variations of carbonates system variables during summer, which reproduce the model. These results are explained in the section 3.2 L280-285 of the MS.

As we did not experiments upwelling events with model, we did not take into account the surface water enrichments by nutrients and TA.
Concerning the riverine inputs scenarii, we decide to focus on nitrate and alkalinity supply. In fact the model simulates the DIC increases, as is observed, which highlight that the carbonate system module is well resolved.

2.4 Code

The code is provided on Zenodo and is easy to download. No reference to this manuscript is given on the model's entry page on Zenodo though. I have not tried to compile the code but only browsed through it as I was interested in getting at least some basic information about the new carbonate system model announced in the title. The code is commented, but most of the comments are unfortunately in French. This is especially annoying for the `Makefile` and the initialisation file `BIO/config.ini` which cannot be understood without a good proficiency in French. No user manual is provided, neither on the Zenodo page nor as a Supplement to the paper.

Reply: Yes, we agree to put comments of the "Makefile" and "config.ini" in English and to add an user manual as a Supplement.

3 Technical comments

Throughout the paper: please always specify which pH scale is used for reporting the data and model results (in tables, on graphs, etc.)

Reply: As suggested by the reviewer at the section of "numerical model description" we add the information that we use the total pH scale (L140). In this way we do not have to add "pH total scale" in all tables and figures.

p. 1, l. 5: is co-author "Irène Remy-Xueref" not actually "Irène Xueref-Remy"? (in the reference section at least the name is spelled that way and that is also the name registered in the submission system)

Reply: We corrected this mistake.

p. 1, l. 18: "22 states variables" should read "22 state variables"

Reply: We corrected as suggested.

p. 1, l. 33: "2018, May to 2019, May" should read "May 2018 to May 2019"

Reply: We corrected as suggested.

p. 2, ll. 42–43: this is unclear. I would not range the biological pump among the physical ones. But it is not sure what is meant here by "physical" pumps.

Reply: We agree with the reviewer we corrected as following L40-42:
"In the ocean, the main processes regulating CO_2 exchanges between the atmosphere and sea are the solubility pump and the biological pump":

p. 2, l. 54: "dynamic" should read "dynamics"

Reply: We corrected as suggested.

p. 2, l. 54: Why only "amplify"? A priori, the forcings could just as well attenuate or reduce acidification.

Reply: We agree with the reviewer we corrected as following L53-54:
"Moreover, these forcings could affect the carbonate chemistry dynamics and amplify or reduce the acidification in coastal zones"

p. 2, l. 56: “At a global scale” should read “At the global scale”

Reply: We corrected as suggested L56.

p. 2, l. 58: “as a net sink or source” may be more appropriate.

Reply: We corrected as suggested L58.

p. 2, l. 63: ‘MacKenzie” should read “Mackenzie” (also misspelled in the bibliography)

Reply: We corrected as suggested.

p.2, ll. 75–76: “strong winds events” should read “strong wind events”

Reply: We corrected as suggested.

p. 3, l. 86: “implemented within” should read “implemented into”

Reply: We corrected as suggested.

p. 3, l. 95: Please delete “inhabitants” (“a population of ca. 1 million” is sufficient).

Reply: We corrected as suggested.

p. 3, l. 97: “winds conditions” should read “wind conditions”

Reply: We corrected as suggested.

p. 3, l. 101: “intrudes in the BoM” should read “intrudes the BoM” or “intrudes into the BoM”

Reply: We corrected as suggested.

p. 3, ll. 103–104: “diverse anthropogenic forcing” should read “diverse anthropogenic forcings”

Reply: We corrected as suggested.

p. 3, l. 106: delete “city”

Reply: We corrected as suggested.

p. 3, l. 113: “modeling platform” should read “platform” (there is no need to repeat the “modeling”)

Reply: We corrected as suggested.

p. 3, l. 113: The paper cited (Baklouti et al., 2006a) is not adequate, as far as I can see. The companion paper Baklouti et al. (2006b), which describes the platform would be more appropriate. Baklouti et al. (2006a) review mechanistic formulations for key processes that control phytoplankton dynamics and present a generic model, less so the platform. Please check this.

Reply: We corrected as suggested.

p. 4, ll. 129–134: The TA production and consumption rates are stated in a very imprecise way here. As such these statement do not make much sense. It should be specified what are the references for the stated TA changes (e.g. TA decreases by two moles for each mole of $CaCO_3$ precipitated, and by x moles for each mole of XY assimilated by phytoplankton, etc.)

Reply: We corrected as following L145-151:
“Based on the review of Middelburg (2019), it is considered that: (i) TA decreases by 2 moles for each mole of $CaCO_3$ precipited, by 1 mole for each mole of ammonium nitrified, by 1 mole for each mole of ammonium assimilated by phytoplankton, and TA increases by 2 moles

for each mole of $CaCO_3$ dissolveld, and by 1 mole for each mole of organic matter mineralized by bacteria in ammonium (See Appendix A Tab. A2)”

p. 4, l. 132: “when bacteria mineralized” should read “when bacteria mineralize”

Reply: We corrected as suggested.

p. 4, l. 147: please delete “However” which does not make sense here.

Reply: We removed as suggested.

p. 4, l. 148: “model results” can be compared with the observations, not the model itself.

Reply: We corrected as suggested.

p. 5, l. 161: “winds specific conditions” should read “wind-specific conditions”

Reply: We corrected as suggested.

p. 6, l. 206: “contains a low value of WSS” – not sure what this could possibly mean. “a low value of WSS” should anyway read “a low WSS” as the last ‘S’ stands for ‘score,’ which is a value.

Reply: We corrected as suggested L224-225:
“The model does not catch the two aforementioned maxima of chlorophyll, and it contains a low WSS and a strong bias (0.37 and +0.22 mg m^{-3}, respectively - Tab. 2).”

p. 6, l. 214: “calculates a WSS value of 0.69” better had to read “yields a WSS of 0.69”

Reply: We modified this sentence as following L234-236:
“The statistical analysis calculated a mean bias of +23 µatm, and a WSS of 0.69 (Tab. 2).”

p. 6, l. 223: “seasonal dynamic” should read “seasonal dynamics”

Reply: We corrected as suggested.

p. 7, ll. 257–262: I am quite surprised about this. I would expect that upwelling events not only bring up cold water, but also nutrient, DIC and TA rich waters. Unfortunately, the model description does not explain how the upwelling events are represented. Could you please elaborate on this.

Reply: In this study we did not experiments the impact of an upwelling events (with a decrease of temperature). We evaluate the impact of different forçings: the temperature, wind, intrusion of nutrients, alkalinity, and atmospheric CO2.
As we did not experiments upwelling events with model, we did not take into account the surface water enrichments by nutrients and TA.

p. 8, l. 281: “diatoms” should read “ diatoms’ ” (genitive)

Reply: We corrected as suggested.

p. 8, l. 295: “in-gassing” should read “absorption” or “uptake”

Reply: We corrected as following L317-319:
“Depending on the gradient of CO_2 *between seawater and the atmosphere, strong wind speeds will favor either the emission or uptake of* CO_2 *(Figs. 6B & E).”*

p. 8, l. 295: “variability” at which time scales?

Reply: We modified as following LXX:
“The seasonal variability of atmospheric CO_2 *concentrations at the urban site …”..*

p. 9, l. 329: “weaker” should read “lower”

Reply: We corrected as suggested.

p. 9, l. 354: I think that “counteracting” is more appropriate than “counterbalanced” at this point

Reply: We corrected as suggested.

p. 12, l. 424: “Environnenemnts” should read “Environnements”

Reply: We corrected as suggested.

p. 12, l. 432: “takes part” should read “is part

Reply: We corrected as suggested.

p. 12, l. 434: “Agence” should read “Agency”

Reply: We corrected as suggested.

p. 12, l. 434: “from European” should read “from the European”

Reply: We corrected as suggested.

p. 12, l. 434: “used in this paper” should read “presented in this paper”

Reply: We corrected as suggested.

Appendix: Details of resolution of carbonate system module

Details of resolution of carbonate system module

1. Calculation of carbonate systems constants:

The constant are calculate in total pH scale

- Conversion of DIC and TA in mol kg^{-1}

$DIC = DIC.\rho_{eau}$ and $TA = TA.\rho_{eau}$

- TF from Riley (1965) in mol.kg^{-1}:

$$TF = \frac{0.000067}{18.998} . \frac{S}{1.80655}$$

- TS from Morris and Riley (1966) in mol.kg^{-1}:

$$TS = \frac{0.14}{96.062} . \frac{S}{1.80655}$$

- Concentration I from the DOE handbook, Chapter 5, p. 13/22, eq. 7.2.4:

$$IonS = \frac{19.924 * \mathrm{S}}{1000 - 1.005 * \mathrm{S}}$$

- Concentration Total borate from Uppström (1974) in mol.kg^{-1}:

$$TB = \frac{0.000416.S}{35}$$

- KS constant of HSO$_4$dissolution from Dickson (1990a) in mol.kg^{-1}:

$$KS = \frac{-4276.1}{T_{(K)}} + 141.328 - 23.093 * \log\left(T_{(K)}\right) + \left(324.57 - 47.986 * \log\left(T_{(K)}\right) - \frac{13856}{T_{(K)}}\right) * Ions^2\text{-}$$

$$KS = KS + \left(-771.54 + 114.723 * \log\left(T_{(K)}\right) + \frac{35474}{T_{(K)}}\right) * Ions + \frac{-2698}{T_{(K)}} * Ions^{1.5} + \frac{1776}{T_{(K)}} * Ions^2\text{- -}$$

$$KS = e^{KS} * (1 - 0.001005 * S)$$

- KF constant of HF formation from Dickson and Riley (1979) in mol.kg^{-1}:

$$KF = e^{\frac{1590.2}{T_{(K)}} - 12.641 + 1.525 * Ions^{1.5}} * (1 - 0.001005 * S)$$

- pH scale conversion factors:

$$\mathrm{SWStoTOT} = \frac{1 + \frac{TS}{KS}}{1 + \frac{TS}{KS} + \frac{TF}{KF}} \text{ and } FREEtoTOT = 1 + \frac{TS}{KS}$$

- KB constant from Dickson (1990b) this is in total pH scale in mol.kg^{-1}

$$KB = (-8966.9 - 2890.53 * S^{\frac{1}{2}} - 77.942 * S + 1.728 * S^{\frac{3}{2}} - 0.0996 * S^2)/T_{(K)}$$

$$KB = KB + 148.0248 + 137.1942 * S^{\frac{1}{2}} + 1.62142 * S + (-24.4344 - 25.085 * S^{\frac{1}{2}} - 0.2474 * S) * \log(T) + 0.053105 * S^{\frac{1}{2}} * T$$

- $K0$ constant of CO$_2$ solubility from Weiss (1974) in mol.kg^{-1}atm^{-1}:

$$K0 = \exp\left(-60.2409 + 93.4517 * \frac{100}{T_{(K)}} + 23.3585 * \log\left(\frac{T_{(K)}}{100}\right) + \mathrm{S} * \left(0.023517 - 0.023656 * \frac{T_{(K)}}{100} + 0.0047036 * \left(\frac{T_{(K)}}{100}\right)^2\right)\right)$$

- Ke: produit ionique de l'eau from Millero (1995), this is in SWS pH scale (mol.kg^{-1})^{2} :

$$Ke = \exp(\frac{-13847.26}{T_{(K)}} + 148.9802 - 23.6521 * \log\left(T_{(K)}\right) + \left(-5.977 + \frac{118.67}{T_{(K)}} + 1.0495 * \log\left(T_{(K)}\right)\right) * S^{1/2} - 0.01615 * S)$$

$Ke = Ke * SWStoTOT$, in total pH scale in mol.kg^{-1}

- $K1$ and $K2$ from Lueker et al., (2000) these are in total pH scale in mol.kg^{-1}:

$$K1 = 10^{\frac{-3633.86}{T_{(K)}}+61.2172-9.6777*\log\left(T_{(K)}\right)+0.011555*S-0.0001152*S^2}$$

$$K2 = 10^{\frac{-471.78}{T_{(K)}}+251.929-3.16967*\log\left(T_{(K)}\right)+0.01781*S-0.0001122*S^2}$$

- Kca for calcite from Mucci (1983) this is in (mol.kg^{-1})^{2}:

$$Kca = 10^{-171.9065-0.077993*T_{(K)}+\frac{2839.319}{T_{(K)}}+71.595*log10\left(T_{(K)}\right)+(-0.77712+0.0028426*T_{(K)}+\frac{178.34}{T_{(K)}}*S^{\frac{1}{2}}-0.07711*S+0.0041249*S^{1.5}}$$

- Ca^{2+} concentration Riley and Tongudai (1967) in mol.kg^{-1}:

$$Ca = \frac{0.02128}{40.087} * \frac{S}{1.80655}$$

- The constant are corrected by pressure:

$R = 83.1451$ in ml.bar^{-1}K^{-1}mol^{-1} and $P_{bar} = 1\ bar$

$$lnK1fac = \frac{\left(25.5-0.1271*T_{(°C)}+0.5*\left(\frac{-3.08+0.0877*T_{(°C)}}{1000}\right)*P_{bar}\right)*P_{bar}}{R*T_{(K)}}; K1 = K1 * e^{lnK1fac}$$

$$lnK2fac = \frac{\left(15.82-0.0219*T_{(°C)}+0.5*\left(\frac{1.13+0.1475*T_{(°C)}}{1000}\right)*P_{bar}\right)*P_{bar}}{R*T_{(K)}}: K2 = K2 * e^{lnK2fac}$$

$$lnKBfac = \frac{\left(29.48-0.1622*T_{(°C)}+0.002608*T_{(°C)}{}^2+0.5*\left(\frac{-2.84}{1000}\right)*P_{bar}\right)*P_{bar}}{R*T_{(K)}}; KB = KB * e^{lnKBfac}$$

$$lnKefac = \frac{\left(20.02-0.1119*T_{(°C)}+0.001409*T_{(°C)}{}^2+0.5*\left(\frac{-5.13+0.0794*T_{(°C)}}{1000}\right)*P_{bar}\right)*P_{bar}}{R*T_{(K)}}; Ke = Ke * e^{lnKefac}$$

$$lnKFfac = \frac{\left(9.78-0.009*T_{(°C)}+0.0009429*T_{(°C)}{}^2+0.5*\left(\frac{-3.91+0.054*T_{(°C)}}{1000}\right)*P_{bar}\right)*P_{bar}}{R*T_{(K)}}; KF = KF * e^{lnKFfac}$$

$$lnKSfac = \frac{\left(18.03-0.0466*T_{(°C)}+0.000316*T_{(°C)}{}^2+0.5*\left(\frac{-4.53+0.009*T_{(°C)}}{1000}\right)*P_{bar}\right)*P_{bar}}{R*T_{(K)}}; KS = KS * e^{lnKSfac}$$

$$lnKcafac = \frac{\left(48.76-0.5304*T_{(°C)}+0.5*\left(\frac{-11.76+0.3692*T_{(°C)}}{1000}\right)*P_{bar}\right)*P_{bar}}{R*T_{(K)}}; Kca = Kca * e^{lnKcafac}$$

- Calculation of Fugacity factor:

We suppose that the pressure is at one atmosphere or close to it (Weiss, 1974):

$Patm = 1.01325\ bar$

$delta = 57.7 - 0.118 * T$ in cm^{3}mol^{-1}

$b = -1636.75 + 12.0408 * \mathrm{T} - 0.0327957 * T^2 + 3.16528 * 0.00001 * T^3$ in cm^{3}mol^{-1}

$$FugFac = exp^{\frac{(b+2*delta)*Patm}{R*T}}$$

2. Resolution of carbonate system

To resolve the carbonate system we calculate the $deltapH$, which is the difference of pH between two iterations. We initialize the run imposing a pH value of 8. Bellow the code details of pH and pCO2 determination:

```
if $(nbiter < 1.)\ pH = 8$
$pHtol = 0.001$ !tolerance for iterations end
$deltapH = pHtol + 1$
do while $(abs(deltapH) > 0.0001)$
    $H = 10^{-pH}$
    $Denom = H^2 + K_1.H + K_1.K_2$
    $CAlk = DIC.K_1.(\frac{H + 2.K_2}{Denom})$
    $BAlk = \frac{TB.KB}{KB + H}$
    $OH = \frac{Ke}{H}$
    $FreetoTot = 1 + \frac{TS}{KS}$
    $Hfree = \frac{H}{FreetoTot}$
    $HSO_4 = \frac{TS}{1 + \frac{KS}{Hfree}}$
    $HF = \frac{TF}{1 + \frac{KF}{Hfree}}$
    $Residual = TA - CAlk - BAlk - OH + Hfree + HSO_4 + HF$
    $Slope = DIC.H.K_1.(H^2 + K_1.K_2 + 4.H.K_2)$
    $Slope = \frac{Slope}{Denom^2} + OH + H + \frac{BAlk * H}{KB + H}$
    $Slope = \log10 * \mathrm{Slope}$
    $deltapH = Residual/Slope$ ! this is Newton's method
    do while $(abs(deltapH) > 1)\ deltapH = \frac{deltapH}{2}$ ! to keep the jump from being too big
enddo
$pH = pH + deltapH$ !Is on the same scale as K1 and K2 were calculated, i.e. total pH scale
$pCO_2 = \left(\frac{DIC*H^2}{H^2+K1*H+K1*K2}\right) * \frac{10^6}{K0*FugFac}$ ! in µatm
$CO_2 = \frac{DIC*10^6}{1+\frac{K1}{H}+\frac{K1*K2}{H^2}}$
$HCO_3 = \frac{K1 * CO_2}{H}$
$CO_3 = \frac{K2 * HCO_3}{H}$
$Omega = \frac{Ca * CO_3 * 10^{-6}}{Kca}$
```