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Interactive comment on "A data-model synthesis to explain variability in calcification observed during a CO_2 perturbation mesocosm experiment" *by* Shubham Krishna and Markus Schartau

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We thank Referee # 2 for the valuable feeback. We will consider most of referee's suggestions for revising our manuscript. One suggestion is to significantly reduce the size of the manuscript. We understand the referee' s constructive criticism. It corresponds with a concern mentioned by the other referee. We largely agree and think that the manuscript can be shortened considerably. For example, all dynamical model equations (detailed source minus sink terms) can be moved to the Appendix. We also decided to put Sect. (2.3.2, Parameter optimisation procedure) to the Appendix, as this might appear to be too difficult to understand for readers who are not familiar with optimisation problems. Those results that are not directly related to calcification or to the

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build-up of coccolithophore biomass will be sorted out.

We will also consider the referee's suggestion to remove the discussion on CN_{fact}, because we have learned that it would actually require an extended in-depth discussion. This is because a CN_{fact} that is different from *one* does not exactly comply with the model's optimality assumptions applied in this study. We greatly appreciate the referee's critical evaluation of our discussion on CN_{fact}. Some figures will be removed from the results and discussion sections. We will, as suggested, combine Figs. (3 and 4), although we prefer plotting the cumulative probability distributions rather than showing the probability densities (see response to specific comment 8). Parts of the conclusion section will be rewritten.

General comments by anonymous Referee #2:

Comment 1: I miss the ecological implications of the findings that have surfaced thanks to the model. For instance, the conclusions should not simply rephrase the modeling aspects, but discuss the ecological implications of the modeling study, or the consequences for future setups of such mesocosm studies.
Author's response: We agree with Referee # 2. In our conclusion section we have not sufficiently stressed the ecological implication of our study and we may also bring forward some general suggestions with respect to the design of future mesocosm "perturbation" studies. In a revised version we will have an extra paragraph added to the conclusion section. The additional paragraph (shown in red) could read:

" An analysis of data of a mesocosm experiment is often approached by first grouping individual mesocosms according to the level of perturbation (e.g. the level of DIC added). In some cases, such apparently self-evident approach may not help to reveal some basic phenomenon. For a meaningful data analysis the mesocosms need

not be exclusively differentiated by the different levels of perturbation but may first be sorted by major differences between relevant response signals, as done with respect to the magnitude of calcification in our study (e.g. differentiating between LC, MC, and HC). In mesocosm experiments these differences in responses are likely associated with variations in initial conditions.

The results of our data-model synthesis show that the initial relative abundance of coccolithophores and the prevailing physiological acclimation states drive the bloom development and determine the amount of calcification in the mesocosms. Small variations of these two initial factors between the mesocosms can generate differences in calcification that are larger than the change in calcification induced by OA. In spite of this difficulty, a CO_2 response signal may still be identifiable, as long as mesocosms that reveal strongest similarities (with respect to initial composition of plankton and their physiological state) are not used as replicates for similar CO_2 conditions (perturbations). Instead, mesocosms with similar initial conditions should be exposed to different levels of OA. Such favourable starting conditions were met in the mesocosm experiment described in Engel et al. (2005) and Delille et al. (2005).

An alternative approach to setting up replicate mesocosms (being subject to the same level of perturbation) is to gradually increase the level of perturbation for a series of mesocosms. This way a gradient of different perturbation levels is introduced. The advantage then is that mesocosms that have been collated according to e.g. lowest and highest response signals (or likewise according to similarities in initial conditions) may then be separately analysed with respect to their responses to the individual levels of perturbation. ”

Comment 2: As a way to reduce the paper in size, I would remove all figures starting from Fig. 11 – and also significantly reduce (or remove) the corresponding text.

Author’s response: In principle, we see that figures can be remove and we will do so

for a revised version of our manuscript. However, to remove all figures starting from Fig. (11) would not be helpful. Some figures are needed to document our findings and to further show the credibility of our model results.
We suggest removing the following figures: 1) Fig. (6, concentrations of dCCHO and TEPC), 2) Fig. (9, ensembles of medium calcification solutions), 3) Fig. (15, fast build-up of photoautotrophic biomass in MC solutions). We find Fig. (14) to be important for the discussion of model bias in PON (exponential growth phase). Figs. (16 and 17) provide relevant information about the i) underestimated CO_2 effect, and the ii) relation between resolved CO_2 effect and the full range of variability explained.
Figs. (3 and 4) will be merged, which was suggested by the referee, see response to specific comment (8) below.

Comment 3: I would also remove the lengthy CN_{fact} discussion (and the corresponding figures 6 and 7, which are difficult to interpret).
Author's response: We will remove Fig. (6) and we will revise text to have the discussion on CN_{fact} entirely removed, as this would actually go beyond the scope of the study addressed here. Figure (7) will be simplified, by excluding variations of CN_{fact}, and by removing results of the medium calcification (MC) case. We want to retain Fig. (7), because it documents some novel model behaviour with respect to how calcification is simulated in our model approach. We compare this ratio with results from Barcelos e Ramos et al. (2010), which gets somewhat lost in the discussion Sect. (4.1). With the removal of the discussion of Fig. (6) it will become easier to explain and refer to Fig. (7).

Specific comments by anonymous Referee # 2:

Specific comment 1: Symbol θ used but not explained.
Author's response: The symbol θ is the chlorophyll-to-carbon ratio (listed in Table 1). We will introduce θ in the text. The revised text will be moved to the Appendix, where the mathematical notation of the model equations is introduced.

Specific comment 2: Equation 13, I would have expected to see zooplankton excretion here.
Author's response: We thank the referee for this very thoughtful comment. We realised that we did not state our assumptions in this respect. First of all, we note that it is not a typo in the equations. In our model we are resolving the nitrogen flux of zooplankton excretion but we are eventually not resolving any corresponding net change in TA (total alkalinity). This is because we cannot really differentiate between the excretion of ammonium (NH_4^+) and of nitrate (NO_3^-) and nitrite (NO_2^-). The excretion of one mole NH_4^+ would increase TA by one mole, whereas the excretion of one mole NO_3^- or NO_2^- would decrease TA by one mole. In other words, we indirectly impose that excreted N does not include urea and we may assume that half of the N excretion by zooplankton is NH_4^+ and the other half is NO_3^- and NO_2^-, which would introduce a net TA change of zero.
For N assimilation during the exponential growth phase we know that it is primarily driven by the uptake of NO_3^- and NO_2^- (due to initial conditions), and the TA change due to NH_4^+ uptake can be neglected. During the post-bloom period we may still have some algal growth, albeit at very low rates, that can be based on the utilisation of NH_4^+. In the end, we expect the error because of a neglect of the net TA change induced by zooplankton excretion to be small and limited to the last days of the simulation period.

Specific comment 3: Page 13-14, I do not understand how the three simulated mesocosms can be used to estimate data variances (R_i) for DIC, as this differs for each mesocosm?

Author's response: In our text we did not explain this in detail. However, we realised that it is necessary to do so. Briefly, for the derivation of the standard errors we considered the differences (offsets) between the mean *initial* DIC concentrations of the different CO_2 treatments. DIC concentrations of those mesososms that were initially exposed to high CO_2 (DIC) concentrations are "offset"-corrected so that their initial mean DIC matches the initial mean of the present day DIC concentrations. Mesocosms of the low CO_2 treatment were adjusted likewise. In this manner, all initial mean DIC concentrations have become identical, but changes and variations (between the mesocosms) with respect to these mean values remain. Thus, variances of the respective LC, MC, and HC mesocosms can be calculated after applying these (two) offset corrections to all DIC data of the high- and low CO_2 treatements. Eventually, individual standard errors for the LC, MC, and HC mesocosms are derived for all sampling dates. Note that the correlations are computed without any differentiation between LC, MC, and HC mesocosms.

Specific comment 4: Page 15, line 2-3: As far as I understand, the proposal distribution is adapted by the AMH algorithm. Thus, the Hessian is used only as the initial proposal.

Author's response: Yes, this is correct. To clarify this we will revise the text in our revised version of manuscript. The new text will read:

" The standard deviation information required for generating the initial proposal (Gaussian) distribution in the AMH algorithm is derived from the diagonal elements of Hessian matrix. We approximated the diagonal elements of the Hessian with finite

central differences, as described in e.g. Matear (1995), Kidston et al. (2011), and in Kreus and Schartau (2015). To do so we imposed an incremental step size of 1% variation to the respective parameter values. ”

Specific comment 5: Page 1, line 18: I do not understand what is meant with "optimal" mass flux estimates, as there are two completely different optimisations: one for the data assimilation (DA), one for the optimal resource allocation in phytoplankton.
Author's response: By “optimal” mass flux estimates we meant the best solution estimated by our data assimilation approach. To avoid any confusion we suggest changing it to “optimised” mass flux estimates.

Specific comment 6: Why is the Chl content not added here?
Author's response: There is no particular reason. We will refine Fig. (2) by adding chlorophyll as additional variable to the respective compartments.

Specific comment 7: Cumulative plots are difficult to interpret. I would prefer to see the actual probability distributions instead. Also, the figs 3 and 4 could be combined, if the three calcification scenarios for each parameter would be put in the same figure rather than in 3 of them.
Author's response: We agree that Figs. (3 and 4) can be combined. However, we do not think that it is better to show the probability densities instead of the cumulative probability distributions. In the end, the cumulative probability distributions are used to derive lower and upper credibility limits of the parameter estimates. Furthermore, if we would prepare the figure with probability densities we would need to resolve differences on the y-axis between the different parameters (i.e. between subplots),

unless we normalise all parameter values. This is not needed when plotting the cumulative probability distributions. The parameter values can then be shown as they are, while all y-axis are the same (between zero and one) so that they can be nicely merged.

Specific comment 8: Fig 8-10: The main difference is in between low and high calcification scenario – Fig 9. Could be removed.
Author's response: Yes, we agree. Main differences are between the HC and LC solutions. Some model solutions of the MC ensemble are close to few solutions of the HC case. Therefore it is not critical to remove current Fig. (9)

All other minor comments and corrections suggested by anonymous Referee # 2 have been implemented.

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