

Interactive comment on “Modelling carbon overconsumption and the formation of extracellular particulate organic carbon” by M. Schartau et al.

M. Schartau et al.

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1 Author’s response to comments of referee #2:

After a careful review, the referee has minor comments on our procedure for approximating posterior probability density distributions. The referee stresses model details that might explain why our model fit to DIC data is not as expected at the final stage of the experiment. The referee also points out that we must refer to the work of Van den Meersche et al. (2004). We consulted the mentioned paper and will refer to it in the discussion. According to the referee’s comments we corrected the respiration formulation in our model. Now, the restoring term does not go below a threshold respiration value

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of 0.01 d^{-1} . In the following we hope to sufficiently respond to the referee's questions.

2 Response to specific comments of referee #2:

2.1 The data assimilation technique

The referee stresses that the bootstrapping approach is computationally more expensive than a Markov Chain Monte Carlo method (MCMC) for approximating posterior error distributions. We agree with the referee in that the bootstrapping needs excessive computational power in order to specify an exact posterior error distribution. In our study, it is not our primary objective to fully resolve the posterior distribution but to obtain parameter estimates for a model configuration capable of simulating carbon overconsumption in conjunction with TEPC formation. Our analysis of the posterior distribution provides ancillary information and helps us to assess our phenomenological model description. We strongly promote the necessity of error- and sensitivity analyses in modelling studies, but we also suggest that one has to find a good balance between the benefit of imparting new knowledge and computational effort. The micro-genetic algorithm provides random samples in the vicinity of our optimised parameter values, similar to MCMC methods. The micro-genetic algorithm searches within the full parameter space while converging and updating the current best estimate. Even when the best solution is identified, the algorithm continues to rescan the entire parameter space, which allows for an approximation of the co-variation matrix, as suggested by the referee. But, the question then becomes how to define the contour level of the cost function for such a subsequent calculations of a full co-variation matrix. Usually this contour level is derived from the effective degree of freedom inherent to the optimisation problem. We do not know the effective degree of freedom. To conclude, we have chosen the bootstrapping approach because we

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intended to learn about the range of uncertainties rather than focusing on great details in the error distribution.

Our description of the probabilities of parameter values is incomplete, as realised by the referee. We follow the referee's suggestion and changed the paragraph. Our prior is uniform within an imposed range of values, and the constant is proportional to the inverse of possibilities (increments) set for the optimisation algorithm.

The referee's advice is correct, the precision can be improved if a gradient search follows the best estimate achieved by the micro-genetic algorithm. We have not applied a gradient-search technique because we must expect that the uncertainties in finding the exact minimum (being a technical problem) are smaller than the range of the spread of individual minima that result from our bootstrapping approach. Thus, we do not expect great benefits by adding gradient search techniques in our study. Improved posterior error estimates can be obtained by either analysing the randomly sampled parameter values in the vicinity of the best estimate, or by extending the bootstrap approach to several hundreds of additional realisations.

Our bias does not only reflect shortcomings of the optimisation algorithm but combines limitations of the chosen metric (cost function), error assumptions for model output, and data. The bias calculated in our study describes whether our error assumptions, based on Gaussian distributions, are appropriate. Having a large bias indicates that our approximation of the standard deviation is poor and that the posterior error distribution is skewed.

We are not able to derive a full-ranked co-variance matrix from observations, since we did not have sufficient replicates (three at best) of all measurements. The inde-

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pendence of data errors is a low-key assumption in order to simplify the resampling of data for our bootstrapping approach. Of course, the original data does contain autocorrelations and it would have been better to add red- instead of white noise. If red noise were introduced then we would have needed to discuss autocorrelations within the system. This issue goes beyond the scope of our study but would be a nice exercise.

2.2 The algal model

1. Modelled changes of the N:C ratio within our phytoplankton compartment do not only depend on luxury uptake of nitrogen but are also sensitive to light availability and bulk Chla concentration. The chosen approach is based on formulations described in Geider et al. (1998). In the case of nitrate shortage, the N:C ratio of phytoplankton converges towards q_{min} , regulating photosynthesis. Thus, photosynthetic rate then becomes rather controlled by nitrogen and light availability. According to the parameterisation used in our study, the rapidity of convergence (down-regulation of the photosynthetic rate) depends on the amount of luxury storage of carbon within the algae.

2. For our study we referred to values listed in Geider et al. (1998), $q_{max}=0.2$ gN/gC and $q_{min}=0.05$ gN/gC. Note that our values are given as molar ratios. We agree with the referee when stating that q_{max} might have been too high for our study. However, we do not intent to improve our fits while imposing parameter values that are difficult to justify. Perhaps our knowledge about minimum and maximum quotas has to be reviewed for cases where these values were derived from POC and PON data. But this remains speculative and we therefore rely on typical values from literature.

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3. With the modified regulation formulation of the nitrogen uptake rate we do have a fast down-regulation at the maximum quota but our step function remains nicely differentiable from below whereas the derivative of the old formulation becomes infinite in the vicinity of Q_{max} . Achieving better smoothness is more important for down-regulating DIN uptake than for down-regulating photosynthetic activity. The maximum photosynthetic rate is linearly decreased when converging towards q_{min} . This is in contrast to the step-like change in DIN uptake near q_{max} .

4. We revised our manuscript and applied changes as suggested by the referee.

2.3 Other model formulations

1. Our formulation of heterotrophic respiration needs to be refined for situations where the heterotrophic community maintains a C:N ratio smaller than Redfield. A better formulation is: Heterotrophic respiration = max(lower threshold, restoring towards prescribed C:N ratio). We did not apply such a formulation during our calculations and therefore expect an error that has to be assessed. We performed new model calculations with a refined formulation (as given above) with a lower threshold value of 0.01 d^{-1} . Differences in DIC remained less than 0.1 percent. The error in the heterotrophic compartment is negligible until day 11. Between day 11 and 15 the model inter-comparison reveals a maximum deviation no more than 9 percent (at 20 mmol C m^{-2} biomass concentration). After day 16 the C:N ratios are always above 6.6 and the deviation reduces to 0.2 percent at day 21. The corrected formulation reduces costs by one unit (e.g. for the best solution $J=256$ instead of 257). One unit reduction in costs falls within our range of uncertainty due to other model limitations. We produced new figures (Figures 2 through 10) with the corrected model formulation, but differences remain so small that they are not detectable by eye, if we use the same scaling for our axes as before. Thus, for our study the improved formulation for

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heterotrophic respiration has a negligible effect on our model results. Nevertheless, we propose to apply the refined formulation.

2. TA changes affected by ammonia are disregarded in our model study because its concentration was around 0.5 mmol m^{-3} , which is less than 2 percent of the initial nitrate concentration, and is negligible against a background of 2440 mmol m^{-3} . Since the effect of ammonia uptake (TA decreases by one mole per mol NH_4 taken up) can become important under different environmental conditions, we become explicit about this in the Appendix section.

2.4 Model fits

We cannot clarify whether carbon overconsumption is underestimated during the final phase of model simulation. The relaxation towards a constant C:N ratio of 6.625 strongly enhances heterotrophic respiration at times when carbon-rich phytoplankton is consumed. We therefore suspected that an overestimation of heterotrophic activity prevails. Since we are not able to specify the deficiency, we rephrased the end of the paragraph: “However, at the end of the simulation period (day 19 through 22), model results show the tendency to either overestimate heterotrophic conditions or to underestimate carbon overconsumption. Given the constraints, we are not able to determine the deficiency that prevails. Both possible scenarios cause elevated DIC and lowered POC concentrations, Figs. 3b and 4a. “

2.5 Technical issues:

We corrected the text in section A6.

The initial value for TEPC concentration was measured and prescribed in the model. All TEPC is regarded as POC. The initial PON concentration (see Table 3) was optimised. Our estimate of the initial PON concentration is transformed to POC by applying the Redfield ratio. TEPC is then added to this initial pool of POC. Because initial biomass is smaller than the initial TEPC concentration we find an initial POC:PON ratio between 12 and 13. Note that the uncertainties are large due to the small biomass concentrations. The actual C:N ratio of phytoplankton fluctuates between 5.8 and 6.2 during the growth phase and then increases to 12 in the post-bloom period. Model results do show small luxury consumption of nitrogen. We have rewritten the paragraph.

If variances are available from observations we apply them but always add a typical background variance (which can be obtained by looking at sensitivities of model results). The overall choice of how one variable relates to the other is not strictly objective. For this reason, we list the variance information explicitly.

The usage of “1” meaning “dimensionless” is common. We leave the decision of which nomenclature to use to the technical editorial office.

We prefer to give bias information in the units of the parameters. In order to relate the goodness of individual estimates to each other, we added a column with the standard deviation divided by the prior range of variation to Table 3.

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