Responses to Reviewer 1

We thank the reviewer for the constructive comments and suggestions which will be very helpful as we revise the manuscript. Below the complete reviewer comments are shown along with detailed responses to each comment (reviewer comments in black, responses in blue font)

Review:

Dear Editor, I read with great interest this manuscript related to the application of an optimization procedure combining satellite and BGC-Argo floats measurements with a biogeochemical model of the Gulf of Mexico. The manuscript is well organized and provides important insight to improve model parameterizations combining state-of the-art sensors data-streams. I found particularly important the results showing the importance of combining chlorophyll and bbp measured by BGCArgo to optimize the model in terms of POC and export. In my opinion it is also important the results that, to a large extent, the optimization procedure carried out on the 1D model can be translated to the 3D model implementation. Therefore, I suggest the publication of this manuscript after minor revisions reported below. My comments are indented in blue.

Minor revisions

Response: We would like to thank the reviewer for the positive assessment and constructive comments.

1. Introduction

Pg2 line 45. because the number of parameters increases exponentially with the number of state variables (Denman, 2003).

I would expect a polynomial [quadratic] not an exponential increase of the parameter number vs state variable number. In fact, Denman (2003) provides a polynomial formula for the increase of fluxes vs state variables and elaborates the estimate of increase of parameters basing on this formula.

Response: Thanks for noting this. As suggested by Reviewer #2, we removed this paragraph in our revised manuscript.

Pg3 lines 68-70. This is especially problematic in oligotrophic regions where the maximum chlorophyll concentration (referred as the deep chlorophyll maximum, DCM) is pronounced near the base of the euphotic zone because of photo-acclimation (Cullen, 2015; Fennel and Boss, 2003).
Could Authors explain better what they mean? In general DCM can appear in mathematical terms even without photo-acclimation (e.g. Varela et al. 1994, Ryabov and Blasius 2008). I suggest Authors to be more specific on this point. Nonetheless, the effect of photo-acclimation mentioned here could produce an enhancement of the DCM feature [already explainable by mechanisms other than photo-acclimation] and could be particularly important for the specific area of the GoM.

References

Varela, R. A., A. Cruzado, and Joaquín Tintoré. "A simulation analysis of various biological and physical factors influencing the deep-chlorophyll maximum structure in oligotrophic areas." Journal of Marine Systems 5.2 (1994): 143-157.

Ryabov, Alexei B., and Bernd Blasius. "Population growth and persistence in a heterogeneous environment: the role of diffusion and advection." Mathematical Modelling of Natural Phenomena3.3 (2008): 42-86.

Response: Here we are referring to the fact that in oligotrophic regions where the deep chlorophyll maximum is pronounced and located relatively deep in the water column, satellite data of surface chlorophyll are insufficient for characterizing the vertically inhomogeneous chlorophyll structure.

Furthermore, in general in the ocean, DCMs are maxima in chlorophyll but not biomass. Typically, there is no biomass maximum associated with the DCM, it is merely an artifact of photoacclimation acting on the exponentially declining light field. This is especially obvious in oligotrophic regions. While it might be true that a biomass maximum coincident with the DCM can be created in mathematical equations as the reviewer suggests (e.g. this is true in an NPDZ model that does not account for photoacclimation), this does not accurately reflect reality.

In our revised manuscript, we changed this sentence into:

"This is especially problematic in oligotrophic regions where the deep chlorophyll maximum (DCM) is relatively deep and hardly observed by the satellite (Cullen, 2015; Fennel and Boss, 2003)."

We also add some brief comments of DCM and biomass maximum (P12 Lines 299-301) when the first time we talked about DCM in our model results to make these two points clearer.

2. Study Region

I would suggest Authors to add information about the recirculation times of the GoM waters with respect to the Atlantic Ocean boundary conditions (BC), this would give an idea on the relevance of the BC in the experiments.

Response: The recirculation times of the open Gulf is relatively long (certainly much longer than our simulation), but we are not aware of a study that specifically looks at this question. We feel that a discussion of recirculation times is well outside of the intended scope of our manuscript. Our treatment of the boundary conditions is consistent with previous modeling studies with the same or a slightly modified version of the same model (Xue et al. 2013, 2016, Yu et al. 2019), hence we are reasonably confident in our set-up.

Xue, Z., He, R., Fennel, K., Cai, W.-J., Lohrenz, S., Huang, W.-J., Tian, H., Ren, W., and Zang, Z.: Modeling pCO_2 variability in the Gulf of Mexico, Biogeosciences, 13, 4359-4377. 2016.

Xue, Z., He, R., Fennel, K., Cai, W.-J., Lohrenz, S., and Hopkinson, C., Modeling ocean circulation and biogeochemical variability in the Gulf of Mexico, Biogeosciences, 10, 7219-7234, doi:10.5194/bg-10-7219-2013. 2013.

Yu, L., Fennel, K., Wang, B., Laurent, A., Thompson, K. R., and Shay, L. K.: Evaluation of nonidentical versus identical twin approaches for observation impact assessments: an ensemble-Kalman-filter-based ocean assimilation application for the Gulf of Mexico, Ocean Science, 15, 1801–1814, https://doi.org/10.5194/os-15-1801-2019, 2019

Moreover it would be interesting to know what are the observed dominant plankton species, or plankton functional types, in the open-ocean part of GoM [pico-phytoplankton and flagellates?]. This could be useful to figure out the implications of the choice of considering one phytoplankton in the model when compared to data.

Response: We chose a one-phytoplankton model because it is simple and thus more likely that the model parameters can be constrained by the limited observations available. If we were using a more complex model, there

would be more uncertain parameters making model optimization much more difficult. In addition, this relatively simple model has been successfully used to study the biogeochemical variabilities (Xue et al., 2013) and CO_2 air-sea fluxes (Xue et al., 2016) in the Gulf of Mexico. The same model has also been used for a number of studies of hypoxia generation in the northern Gulf of Mexico (e.g. Fennel et al. 2011, Yu et al. 2015, Laurent et al. 2017, 2018, Große et al. 2019). While we agree with the reviewer that analyses of model complexity are important and interesting, such a discussion is outside of the intended scope of this manuscript. There are dedicated publications on this (e.g. Kuhn et al. 2019). We believe we are making a novel contribution on a different important topic in this manuscript.

Fennel, K., Hetland, R., Feng, Y., and DiMarco, S.: A coupled physical-biological model of the Northern Gulf of Mexico shelf: model description, validation and analysis of phytoplankton variability, Biogeosciences, 8, 1881–1899, https://doi.org/10.5194/bg-8-1881-2011, 2011.

Große, F., Fennel, K., & Laurent, A.: Quantifying the relative importance of riverine and open-ocean nitrogen sources for hypoxia formation in the northern Gulf of Mexico. Journal of Geophysical Research: Oceans, 124. https://doi.org/10.1029/2019JC015230. 2019.

Kuhn, A. Fennel, K.: Evaluating ecosystem model complexity for the northwest North Atlantic through surrogate-based optimization, Ocean Modelling, https://doi.org/10.1016/j.ocemod.2019.101437, 2019.

Laurent, A., K. Fennel, W.-J. Cai,W.-J. Huang, L. Barbero, and R. Wanninkhof: Eutrophication- induced acidification of coastal waters in the northern Gulf of Mexico: Insights into origin and processes from a coupled physical-biogeochemical model, Geophys. Res. Lett., 44, 946–956, doi:10.1002/2016GL071881. 2017.

Laurent, A., Fennel, K., Ko, D. S., & Lehrter, J.: Climate change projected to exacerbate impacts of coastal eutrophication in the northern Gulf of Mexico. Journal of Geophysical Research: Oceans, 123, 3408–3426. https://doi.org/10.1002/2017JC013583. 2018.

Xue, Z., He, R., Fennel, K., Cai, W.-J., Lohrenz, S., and Hopkinson, C.: Modeling ocean circulation and biogeochemical variability in the Gulf of Mexico, Biogeosciences, 10, 7219–7234, https://doi.org/10.5194/bg-10-7219-2013, 2013.

Xue, Z., He, R., Fennel, K., Cai, W.-J., Lohrenz, S., Huang, W.-J., Tian, H., Ren, W., and Zang, Z.: Modeling pCO2 variability in the Gulf of Mexico, Biogeosciences, 13, 4359–4377, https://doi.org/10.5194/bg-13-4359-2016, 2016.

Yu, L., Fennel, K., Laurent, A., Murrell, M. C., and Lehrter, J. C.: Numerical analysis of the primary processes controlling oxygen dynamics on the Louisiana shelf, Biogeosciences, 12, 2063–2076, https://doi.org/10.5194/bg-12-2063-2015, 2015.

3. Methods

3.1. Biological observations

Pg 5 lines21-22 SeaWiFS (Sea-viewing Wide Field-of-view Sensor), MODIS (Moderate resolution Imaging Spectroradiometer), and MERIS (medium-spectral resolution imaging spectrometer) products.
What about VIIRS? Is it included in the database?, please check.

Response: We checked and confirmed that indeed VIIRS is included in the database. We corrected it in our revised manuscript (P5 Lines 109-112) and thank the reviewer for pointing this out.

Pg 5 line 26 and particulate backscattering
Pg 5 lines 31-32 Satellite estimates were therefore corrected following the regression equation shown in Figure S2a (Figure S1c).
Pg 6 lines 45-48 The bbp700 from the floats is weakly correlated with the satellite estimates (R^2=0.11) and generally lower by a factor of ~0.45 than the satellite estimates (Figure S2b). The bbp700 profiles were therefore multiplied by 2.2 before being converted to bbp470 following the equ. 1.

In one case Authors consider the BGC-Argo the ground truth (Pg 5 lines 31-32) in the other Authors correct BGC-Argo with respect to satellite data (Pg 6 lines 45-48). The procedure seems a bit circular, could Authors explain better this part?
Pg 6 line 44 extent

Response: Chlorophyll and backscatter, regardless of whether they are obtained by satellite or in-situ sensors, are proxy measurements. That means they have to be converted and calibrated before they can be used. Here the BGC-Argo floats provided measurements of chlorophyll fluorescence and the volume scattering function at a centroid angle of 140° and a wavelength of 700nm ($\beta(140^o, 700nm)$ m^{-1} sr^{-1}), i.e. a measure of backscatter. The conversion from fluorescence into chlorophyll concentration was based on the sensor manufacturer's calibration. The conversion into bbp700 was performed by us following Green et al. (2014) and by cross-calibration against existing relationships with POC and phytoplankton biomass (Martinez-Vicente et al., 2013; Rasse et al., 2017). The resulting concentrations of phytoplankton biomass and POC as well as the ratio of chlorophyll to phytoplankton biomass are reasonable (please see figures 4 and 10).

We rewrote these paragraphs and included a more in-depth explanation of this process in our revised manuscript (P5-6 Lines 123-151).

Green, R. E., Bower, A. S. and Lugo-Fernandez, A.: First Autonomous Bio-Optical Profiling Float in the Gulf of Mexico Reveals Dynamic Biogeochemistry in Deep Waters, PLoS ONE, 9(7), 1–9, doi:10.1371/journal.pone.0101658, 2014.

Martinez-Vicente, V., Dall'Olmo, G., Tarran, G., Boss, E. and Sathyendranath, S.: Optical backscattering is correlated with phytoplankton carbon across the Atlantic Ocean, Geophysical Research Letters, 40, 1154–1158, doi:10.1002/grl.50252, 2013.

Rasse, R., Dall'Olmo, G., Graff, J., Westberry, T. K., van Dongen-Vogels, V. and Behrenfeld, M. J.: Evaluating Optical Proxies of Particulate Organic Carbon across the Surface Atlantic Ocean, Frontiers in Marine Science, 4(November), 1–18, doi:10.3389/fmars.2017.00367, 2017.

3.2. 3D Model description

Pg 7 lines 74-75 Medium-Range Weather Forecast ERA-Interim product with a horizontal resolution of 0.125o (ECMWF reanalysis, https://www.ecmwf.int/en/forecasts/datasets/reanalysisdatasets/era-interim).

The resolution reported in the link above for ERA-Interim is 80 km this does not match with the 0.125° (~12 km) reported in the manuscript, could Authors double check?

Response: The resolution of ~80 km is the model grid resolution used by the ERA-Interim's atmospheric model and reanalysis system. However, they also provide their dataset for download in higher (e.g. 0.125°) or coarser resolutions (e.g. 3°) which the original data are interpolated onto. We used the higher-resolution data set as stated in the manuscript.

3.3. 1D Model description

Pg8 line 10-12. The 1D model, which is similar to that used by Lagman et al. (2014) and Kuhn et al. (2015), covers the upper 200 m of the ocean with a vertical resolution of 5 m and is configured at one location in the central Gulf (see Figure 1).

Authors should add some comment about the choice of 5 m vertical resolution. What is the 3D model vertical resolution in the same region of the GoM? Why not taking 1m resolution that probably is the vertical resolution of data acquired by BGC-Argo floats?

Response: There are two main reasons why we chose 5 m. First, the vertical resolution in our BGC-Argo floats is 4-6 meters in the upper 200 m. Second, a 5-m vertical resolution in the 1D model keeps the computational cost reasonable. As stated in sections 3.4 and 3.5 of the manuscript, one parameter optimization experiment ran 36,000 model simulations (30 simulations/generation * 300 generations*4 replications). It took us about one day to run a single parameter optimization experiment and we performed 13 1D optimization experiments in total (A1-A4, B1-B4, C1-C5). This is in addition to all the 3D model runs we performed.

We are confident the vertical resolution is appropriate because we performed sensitivity tests using different vertical resolutions including 10 m, 5 m, 3 m, and 1 m in optimization C4. As shown in Figures 1 and 2 below, the choice of vertical resolution has little impact on model results except for minor jumps in the DCM depth (Figure 1e) and DCM magnitude (Figure 2) when a vertical resolution of 10 m is used.

The 3D model had 36 terrain-following sigma levels with refined resolution near the surface and bottom layers. The vertical resolution in the 3D model varied from a few meters near the surface to ~50 m near the depth of 200 m around the 1D site.

In our revised manuscript, we added comments on the 1D model's vertical resolution as suggested (P8 Lines 200-202).

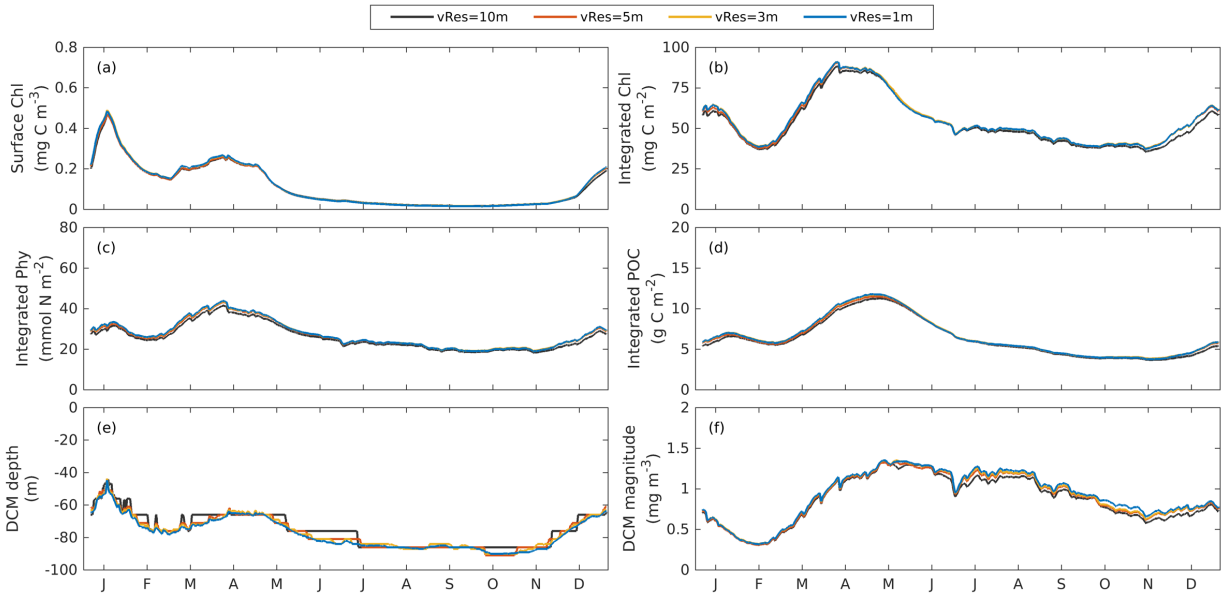

Figure 1. The simulated annual cycle of surface chlorophyll (a), vertically integrated chlorophyll (b), vertically integrated phytoplankton (c), vertically integrated POC(d), and the depth (e) and magnitude (f) of the DCM by using different vertical resolutions.

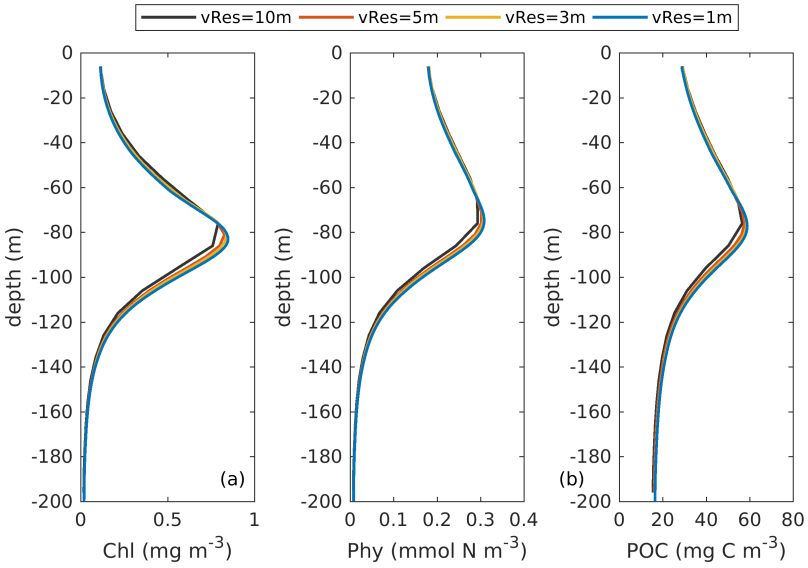

Figure 2. The simulated vertical profiles of chlorophyll, phytoplankton, and POC by using different vertical resolutions.

Pg9 line 13-15. A higher diffusion coefficient (K_{ZI} =max(H^2MLD /400,10))is applied in the turbulent surface layer and a lower diffusion coefficient (K_{Z2} =K_{ZI}/2) is assigned to the quiescent bottom layer.

What is the unit of measure of K1,2, please add this information in the text. If it is m2/s it seems very high, because even with H_{MLD} = 0 → K_{ZI} =10 → $KZ2$ =5. Please, add also unit of measure of H_{MLD}, meters?

Response: The units of K_{Z1} and K_{Z2} are m^2/day. The unit of H_{MLD} is in meters. We added the units as suggested in our revised manuscript (P8 Lines 204-206).

3.4. Parameter optimization method

Pg 11 line 63. and n is the number of base-test pairs including

I suggest to use consisting rather than including that in my opinion is confusing. In fact n accounts exactly to what specified (i.e. base –test pairs etc etc)_and not more.

Response: Revised as suggested.

The range of variability of Wphy spans many orders of magnitude and it is the most sensitive parameter, could Author comment on that?

Response: The range of sinking speeds for organic matter is large, because pico-plankton sink very slowly, if at all, while large detrital aggregates can sink very fast. We used the same range for all sinking speed in the optimization, as reported in Table 1 (for Wphy, WSdet, WLdet), although the speeds for Phy will be in the lower range of the bracket, speeds for SDet in the middle range, and speeds for Ldet in the upper range.

3.5. Parameter optimization experiments

Pg 11 line 69-71. For the parameter optimization of the 1D model, satellite chlorophyll within a 3´3 pixel (12 km´12 km area) around the 1D station and climatological monthly averages of the profiles from the bio-optical floats were used.

Did you considered all the BGC-Argo data available or only the ones near the virtual mooring of your 1D experiment? How you decided the BGC-Argo float to include in the optimization procedure?

Response: We used all BGC-Argo data by averaging all profiles into climatological monthly bins. We did this because 1) the BGC-Argo profiles were sparsely distributed in the Gulf of Mexico and there were few profiles around the 1D site, and 2) the deep Gulf of Mexico is quite homogenous horizontally.

In the revised manuscript, we added statements to make this clearer (P10 Lines 257-259).

Pg 11 line 81-84. Prior tests have shown that the available observations cannot simultaneously constrain the sinking rates of small and large detritus (wSDet and wLDet)Therefore, a constant ratio of 0.1 between these two parameters (wSDet =0.1 wLDet) was imposed and only one of the two was optimized.

I suggest Authors to be clearer: I cannot get why the two parameters cannot be constrained. In general, after you completed your optimization procedure you could perturb the parameter 0.1 (ratio between WsDet and WlDet) to see if it corresponds to a minimum for your metrics F(p) or if there are better values other than 0.1. Or the system is unstable if you don't take 0.1? Please explain.

Response: These two parameters cannot be constrained simultaneously because they can compensate each other: an increase in one parameter can be counteracted by a decrease in the other. This is a well-known and much discussed issue in the parameter optimization literature. Basically, there is no information in the available observations that allows to distinguish between the two. Including both parameters in the optimization will degrade the model's predictive skill. To solve this problem, one can either introduce more independent observations or prior knowledge by, e.g. fixing these parameters to their prior values or defining a link between these parameters. Generally, and also in this case, observations are insufficient to constrain all parameters and prior knowledge about

the parameters has to be included. This is the common approach to address the underdetermination problem of parameter optimization in biological models.

In this study, the ratio of 0.1 was selected based on the prior values of the two parameters. Perturbing and estimating the ratio between two sinking velocities are equivalent to letting both parameters (wSDet and wLDet) into optimization and may degrade model's predictive skills. Without additional information about the depth distribution of Sdet and Ldet, which is not available, the ratio cannot be constrained.

The underdetermination problem and the practice of incorporating prior knowledges is also discussed on P20, L10-28 of our original manuscript.

Pg 12 line 92 please remove *and* from the equation.

Response: Revised as suggested.

4. Optimization of 1D models

General question: how you define the DCM depth in the presented analyses?

Response: In this study, the DCM depth was defined as the depth where the subsurface chlorophyll is at its maximum. The definition of DCM depth was included in our revised manuscript (P12 Lines 300-301).

4.1. Observations and base case

Pg 12. Lines 107-109. Unlike the surface chlorophyll, the vertically integrated chlorophyll as well as the phytoplankton and POC over the upper 200 m tend to be more constant with much less seasonality (Figure 3b-d).

This statement refers to observation? Please specify. Is it possible to add the error bar to the dots of Figure 3 as in the case of Figure 4?

Response: Yes, we are referring to observations which are represented by black dots. We clarified this (P12 Line 295) in our revised manuscript and added the error bar in Figure 3 as suggested.

Pg 12 line 14 in June and gradual shoaling after July (Figure 3e), reflecting the seasonality of the solar radiation.

With the term reflecting Authors mean that there is direct causality or correlation?

Response: We think that there is direct causality between the shoaling of DCM depth and solar radiation. In the oligotrophic regions, the DCM is strongly determined by photoacclimation (Cullen, 2015; Fennel and Boss, 2003). Previous studies based on BGC-Argo floats also suggest that the DCM is mainly light driven and located at the level of a particular isolume (e.g. Mignot et al., 2014; Xing et al., 2018). In our case, with the decrease of solar radiation after July, these isolumes and the DCM would therefore become shallower.

Cullen, J. J.: Subsurface Chlorophyll Maximum Layers : Enduring Enigma or Mystery Solved ?, Annual Review of Marine Science, 7, 207–239, doi:10.1146/annurev-marine-010213-135111, 2015.

Fennel, K. and Boss, E.: Subsurface maxima of phytoplankton and chlorophyll : Steady-state solutions from a simple model, Limnology and Oceanography, 48(4), 1521–1534, 2003.

Mignot, A., Claustre, H., Uitz, J., Poteau, A., D'Ortenzio, F. and Xing, X.: Understanding the seasonal dynamics of phytoplankton biomass and the deep chlorophyll maximum in oligotrophic environments: A Bio-Argo float investigation, Global Biogeochemical Cycles, 28(8), 1–21, doi:10.1002/2013GB004781, 2014.

Xing, X., Qiu, G., Boss, E., & Wang, H. Temporal and vertical variations of particulate and dissolved optical properties in the South China Sea. Journal of Geophysical Research: Oceans, 124. https://doi.org/10.1029/2018JC014880. 2019.

Pg 13 line 18 However, it fails to reproduce the deepening of the DCM in June

This deepening is related to a physical process (change in some environmental regulating factor) or to a biogeochemical process?

Response: This deepening is a result of both physical and biological processes. Firstly, as stated in the reply to the last comment, the increase of solar radiation would make the DCM deeper. Secondly, as the water column becomes more stratified in summer, chlorophyll concentrations in the upper layer will be lower as a result of nutrient limitation, which in turn increases light penetration through the water column and thus causing the DCM to deepen.

4.2. Results of the optimizations
4.2.1 Model-data misfits
4.2.2 Experiment A
Pg 13 line 41-42 The optimal parameter sets (A4, B2, and C4), which are selected based on casespecific misfit from these three groups, will be used in subsequent analyses …

Why Authors decide to use B2 rather than B4 that show a smaller total misfit? Is it better to take a realization with better case-specific misfit or better total misfit?

Response: Firstly, experiments in group B represent the scenario where we only have chlorophyll observations. In that case, we would have no idea about the model misfit for other variables except chlorophyll or the total misfit. Secondly, the case-specific misfit was the criterion that the parameter optimization procedure used to choose the best half population while "killing" the other half. Hence, using B2 rather than B4 as the optimal parameter sets makes sense.

We discussed the choice of B2 in our original manuscript. In realistic parameter optimization applications where only chl and no other observation are available the B2 optimization would be chosen. Revealing this weakness due to insufficient observations can help us to better understand the additional value of BGC-Argo floats and provide some scientific guidance for future parameter optimization studies. This is really the point we are trying to make here.

4.2.3 Experiment B
Pg 14 line 47-49 However, the vertical structure of chlorophyll deteriorates relative to the base case (Figure 4a) because of inappropriate estimates of the initial slope (α=0.0101; see table 2) and the maximum ratio of chlorophyll to carbon (θmax=0.0191; see table 2).

If Authors can judge a-priori that the values for α and θmax resulting from the optimization are not appropriate, why they didn't consider different parameter ranges in the optimization procedure from the beginning, excluding bad values?

Response: Firstly, we have no prior knowledge of these parameters in the Gulf of Mexico and that is why we run parameter optimization to estimate their values. Our comments on these two parameters here were based on the results of our parameter optimization experiments.

Secondly, we feel these two parameters were inappropriate after we compared model results with vertical profiles of chlorophyll and phytoplankton. Since experiment A was designed to represent the scenario where only satellite observations are available, adding the information obtained from the BGC-Argo floats data into experiment A would not be a fair comparison to the other experiments and violate our assumptions of the experiment A.

Pg 14 lines 57-59. A straightforward interpretation is that the addition of subsurface observations reduces the model's degrees of freedom to fit one single observation type (surface chlorophyll).

Does this imply that a model with more parameters (e.g. more phytoplankton species) would fit better?

Response: Here we mean that the addition of subsurface observations yields more constraints on our biological model because the model should fit both surface and subsurface observations simultaneously.

With respect to reviewer's comment, it tends to be true but not always. However, the better fit is often the result of overfitting rather than a true improvement in predictive skill. It is of utmost importance to avoid overfitting. The increased number of parameters in more complex models may increase the risk of degrading model's predictive skills.

Pg15 line 70 In contrast to the observations where detritus dominates POC …

What observation? Please add reference.

Response: Here we referred to our BGC-Argo floats shown in Figure 4. We included reference (P14 Lines 354-356) in our revised manuscript as suggested. And as suggested by the Reviewer #3, we changed this sentence into:

"In contrast to the observations where the phytoplankton's contribution is neglectable (Figure 4), the simulated POC at 200 m is dominated by phytoplankton (49%)"

4.2.4 Experiment C

Pg 15 lines 76-78 As shown in Figure 4a, the annually averaged depth of DCM of 80 m coincides with the observed DCM, primarily because experiment reproduces the deepening of the DCM in summer.

Interesting. Can Authors explain if there is a specific parameter/mechanism that controls this dynamical deepening of the DCM? Or it is a complex combination of parameters values generating this emergent property?

Response: As we mentioned above, the deepening of the DCM in the summer resulted from a combination of increased solar radiation and decreased light attenuation in the upper layer. Since the different experiments here used the same inputs of solar radiation, the deepening of the DCM in experiment C must be a result of changes in parameter values which can influence chlorophyll concentrations and hence light attenuation in the upper layer. To illustrate this, we performed sensitivity simulations where we used the optimal parameters from experiment C but set each optimized parameter, one at a time, to its prior value. As shown in Figure 3, the optimization induced changes in large detritus remineralization rate (r_{LD}), half-saturation for NH4 uptake (K_{NH4}), and large detritus sinking velocity (w_{LDet}) can have large impacts on chlorophyll concentrations and the depth of DCM.

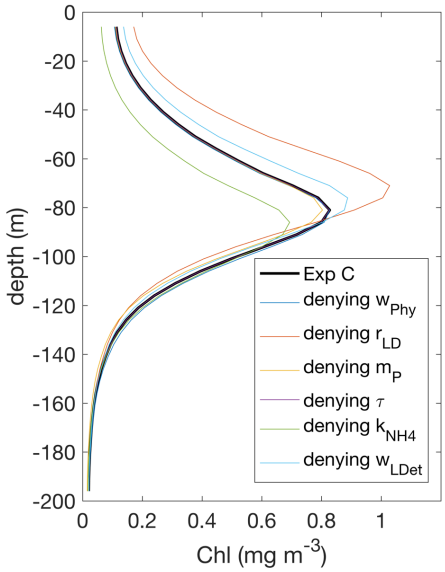

Figure 3: Vertical distributions of simulated chlorophyll from different sensitivity tests.

5. 3D biogeochemical model

Could Author explain better the manual correction described at pg 17 lines 24-25? If they consider the corrected values more realistic why they didn't narrowed the parameter variability range in the optimization experiment? Or the 1D vs 3D implementations do not allow this?

For example, is there a simple explanation for the need to set KNH4 to 0.01 in the 3D experiments? It would be useful for readers interested in applying this methodology in other areas.

Response: We did manual modifications because when the resulting parameters were directly applied, the model-data agreement in 3D models was not as well as in 1D models in some respects, but the most important features were well preserved. In experiment C, chlorophyll concentrations in the upper layer of 3D model were lower than the 1D model and farther away from observations. This might be a result of differences between 1D and 3D models and has been also reported in other studies (e.g. Kane et al., 2011; Hoshiba et al., 2018). However, the depth of the DCM and the non-zero POC concentrations at 200 m with appropriate contributions from each component were well preserved. We therefore did some tests manually by tuning one or two parameters and final set the KNH4 to 0.01 in order to have a better agreement with respect to observations. All of these modifications were based on our tests.

In our case, although the 1D parameter sets could not be used in 3D models directly, they were sufficient to reproduce the main features as in 1D models and largely simplified the following subjective tuning of 3D models by limiting the number of parameters to be adjusted.

We included more explanations for the manual modifications (P16 Lines 400-411) and discussion (P20-21 Lines 522-530) in our revised manuscript.

Kane, A., Moulin, C., Thiria, S., Bopp, L., Berrada, M., Tagliabue, A., Crépon, M., Aumont, O. and Badran, F.: Improving the parameters of a global ocean biogeochemical model via variational assimilation of in situ data at

five time series stations, Journal of Geophysical Research: Oceans, 116, 1–14, doi:10.1029/2009JC006005, 2011.

Hoshiba, Y., Hirata, T., Shigemitsu, M., Nakano, H., Hashioka, T., Masuda, Y. and Yamanaka, Y.: Biological data assimilation for parameter estimation of a phytoplankton functional type model for the western North Pacific, Ocean Science, 14, 371–386, doi:10.5194/os-14-371-2018, 2018.

It would be useful to know how the PP from the model is computed: integrating down till the bottom, considering thee MLD?

Response: The primary production in the 3D models was integrated down to 200 m, consistent with the primary production obtained from the 1D models. There is not enough available light below 200 m for photosynthesis to occur, therefore cutting off at 200 m yields the same values of integrated primary production as integration down to the seafloor would. As suggested, we stated this in our revised manuscript (P17 Lines 445).

6. Discussion

6.1 Trade-offs between different observations for parameter optimization

In this section Authors use a number of times the following terms poorly constrained, weakly constrained and unconstrained, un-optimized fields, not optimized but well defined. Some definitions can be grasped from section 3.5. In my opinion it would make things more simple to have the formal definition of these terms and to know if, in same cases, they are equivalent/synonym.

Response: The poorly constrained and weakly constrained parameters are synonymous, meaning that they cannot be constrained in confidence. In our study, it can be simply understood that their estimates were inappropriate. The unconstrained and un-optimized fields are equivalent meaning that they were not included in the parameter optimization procedure. The not-optimized but well-defined parameters are those parameters which were not included in the parameter optimization but their prior values were coincidently reasonable. As suggested, we tried to simplify the language and included these definitions in our revised manuscript.

Pg 21 lines 36-42 Although this cross-validation at different times and locations may give some indication of overfitting, it cannot determine whether the model reproduces observation through wrong mechanisms because a small misfit of cross-validation can be caused by missing validations of key variables or fluxes, e.g. ignorance of phytoplankton and PP in the experiment B, while a large misfit can be a result of the intrinsic heterogeneity of biological parameters in different times (Mattern et al., 2012) and locations (Kidston et al., 2011), e.g. underestimation of coastal surface chlorophyll in the experiment C.

In my opinion the sentence above is not very easy to follow, could Authors simplify?

Response: As suggested, we revised these sentences into:

"However, even when cross-validation at different times and locations produces large misfits, we cannot conclude that the models reproduce observations through wrong mechanisms. This is because the large misfit can be a result of intrinsic heterogeneity of biological parameters at different times (Mattern et al., 2012) and locations (Kidston et al., 2011)."

Pg21 lines 54-55 On the other hand, counter examples exist where the 3D simulations outperform the 1D model (Hoshiba et al., 2018).

Could Authors explain better this sentence? Outperform with respect to what aspect?

Response: Here we mean that applying parameters obtained from 1D models could result in worse or better fitness in 3D models. For instance, Hoshiba et al. 2018 performed parameter optimization by 1D models and applied the resulting parameters in 3D models. As a result, the 3D model had better fitness than the 1D model with respect to vertical profiles of phytoplankton and nitrate (please see their section 3.4 and Figure 10a,b). As suggested, we clarified this in our revised manuscript (P20 Lines 525-526).

Hoshiba, Y., Hirata, T., Shigemitsu, M., Nakano, H., Hashioka, T., Masuda, Y. and Yamanaka, Y.: Biological data assimilation for parameter estimation of a phytoplankton functional type model for the western North Pacific, Ocean Science, 14, 371–386, doi:10.5194/os-14-371-2018, 2018.

Response to Peter Strutton (Referee #2)

We thank the reviewer for the constructive comments and suggestions which will be very helpful as we revise the manuscript. Below the complete reviewer comments are shown along with detailed responses to each comment (reviewer comments in black, responses in blue font)

Review:

This is a very useful contribution that explains the benefit that models can derive from the incorporation of satellite and BGC-Argo observations. The paper is timely and clearly written. I recommend publication after minor revisions.

Response: We would like to thank the reviewer for the positive assessment and constructive comments.

Specific comments:

The introduction is comprehensive. It could be shortened a bit (the 3rd and 5th paragraphs could mostly be removed) but this is not essential.

Response: Thanks for these suggestions. The 5th paragraph is to show weakness of satellite observations which served as the motivation of this study and is highly related to some main conclusions. We would therefore like to keep it in our revised manuscript. As suggested, the 3rd paragraph was removed.

Methods switch between present and past tense. Also not a big deal, just disconcerting for the reader.

Response: We looked through the whole Methods section and made the tense appropriate in our revised manuscript.

P6 L48: Here and in subsequent equations/text I'm a bit confused. The float and satellite measure bbp700 and bbp670 respectively. So why are we now talking about bbp470? And what is meant by 'validated bbp470'?

Response: We talked about bbp470 because the empirical relationship that we used to estimate phytoplankton and POC was based on bbp470 (please see equ. 2-3). We had to convert measurements of bbp700 and bbp670 to bbp470 based on the equ. 1 before we estimated phytoplankton and POC.

We rewrote the paragraphs about processing the backscatter and made it clearer in our revised manuscript (P5-6 Lines 123-151).

P6 Eq 2 and 3: What are the units of the terms on the LHS? Please be more specific about what 'Phytoplankton' is. I think it's phytoplankton N.

Response: Yes, the phytoplankton and POC were in unit of mmol N m^{-3}. We actually have mentioned it in P6-7 L58-60 in our original manuscript. We also revised and made it clearer here as suggested (P5 Lines 125-127).

P11 L69: Here and in section 3.1, the temporal resolution of the satellite data is not specified. I also think a bit more information here would be useful. How are monthly climatologies of the float profiles created? What distance from the 1D site is considered? Maybe this is described elsewhere and I missed it, but I see the other reviewer asked something similar.

Response: In this study, we used monthly satellite estimates of surface chlorophyll in the parameter optimization. The monthly climatology of float profiles was created by averaging all profiles collected in the Gulf of Mexico into monthly bins. We did this because 1) the BGC-Argo float profiles were sparsely distributed in the Gulf of Mexico and there were insufficient profiles around the 1D site (please see figure 1 in our original manuscript), and 2) the deep ocean part of the Gulf of Mexico is quite homogenous horizontally. As suggested, we included some more description and explanation in our revised manuscript (P5 Line 107 and P10 Lines 256-259).

P14-15: In the sub-section headings, it wouldn't hurt to remind us what experiments A, B and C are. That is 'satellite only' etc.

Response: Agree. Revised as suggested

Figures 3 and 8: Why not just put the parameter labels on the y axes?

Response: Yes, revised as suggested.

For the 3D case, I think it's correct to say that Figure 8 is an average of all model grid cells where the water depth is >1000m. That's a pretty big area. Yes, it's reasonably uniformly low chlorophyll, so one could make the case that this encompasses a contiguous bio-region. But why not choose a smaller box in the middle of the deep part of the basin, and perhaps one from the shelf, to illustrate the model performance? I suspect the latter will not perform as well, but that would still be interesting to know.

Response: To the first point, since the BGC-Argo float profiles are sparsely distributed in the deep part of the Gulf of Mexico (please see Figure 1 in our original manuscript), choosing a smaller box would mean that much fewer float profiles are available for the model-data comparison. Also, since the region is quite homogenous horizontally, we feel it is appropriate to average over all. In Figure 4, we show the interquartile range of the profiles in space and time (black bars). These are very similar if calculated only for July. Thus, the error bars in Figure 4 give a good indication of the spatial variability. We added some comments about this in the revised manuscript (P17 Lines 425-427).

To the second point, the BGC-Argo floats were deployed only in the deep part of the Gulf, hence no float profiles are available on the shelf. However, we agree that it would be interesting to show the validation in smaller boxes from the deep ocean and shelf, and we included this comparison with satellite surface chlorophyll in the supplementary of our revised manuscript.

The results proceed in a logical fashion through the different experiments, 1D and 3D. The presentation of the results is clear and concise.

Response: Thank you, we really appreciate this comment.

In a paper like this, readers will likely be looking for a clear recommendation: Which of the three options should they choose? I think the conclusions do a good job of summarizing the recommendations and the figures represent what's lost if it's not possible to implement the best case scenario.

Response: Thank you, we are happy to hear this.

Responses to Mara Freilich (Reviewer 3)

We thank the reviewer for the constructive comments and suggestions which will be very helpful as we revise the manuscript. Below the complete reviewer comments are shown along with detailed responses to each comment (reviewer comments in black, responses in blue font)

Review:

This manuscript presents a very well developed and well described parameter optimization process for biogeochemical models using available sea surface and profile observations. The authors show that a model parameterized with both surface chlorophyll from satellite and BGC-Argo profiles of chlorophyll and POC best represents the available observations of ecosystem state and fluxes. The authors demonstrate that the parameter choice has important implications for carbon cycling and export.

Comments:
2. Study Region
This section is very useful as an orientation to the region. Since one of the major objectives of the study is to analyze carbon export, it would be useful to include more in this section about what is known about carbon export in the Gulf of Mexico.

Response: We would like to note that the major objective of this study is to evaluate the trade-offs between different observation types for biological model validation and parameter optimization. Our model-data comparison of carbon export is to illustrate the model performance and additional value brought by BGC-Argo profiles to parameter optimization. Studying the carbon export in the Gulf of Mexico is not within the intended scope of this study.

3. Methods
p. 6, Line 147: Earlier in this section, the satellite chlorophyll was adjusted to the float chlorophyll, but here the float backscattering is adjusted to the satellite backscattering. Why is this? These adjustments may have important implications for the POC profiles and partitioning of POC between phytoplankton, zooplankton, and POC. The reasoning for and implications of this choice should be explained.

Response: Chlorophyll and backscatter, regardless of whether they are obtained by satellite or in-situ sensors, are proxy measurements. That means they have to be converted and calibrated before they can be used. Here the BGC-Argo floats provided measurements of chlorophyll fluorescence and the volume scattering function at a centroid angle of 140° and a wavelength of 700nm ($\beta(140^o, 700nm)$ m-1 sr-1), i.e. a measure of backscatter. The conversion from fluorescence into chlorophyll concentration was based on the sensor manufacturer's calibration. The conversion into bbp700 was performed by us following Green et al. (2014) and by cross-calibration against existing relationships with POC and phytoplankton biomass (Martinez-Vicente et al., 2013; Rasse et al., 2017). The resulting concentrations of phytoplankton biomass and POC as well as the ratio of chlorophyll to phytoplankton biomass are reasonable (please see figures 4 and 10).

We rewrote these paragraphs and included a more in-depth explanation of this process in our revised manuscript (P5-6 Lines 123-151).

Since this comment is similar to comments by Reviewer #1 under 3.1, we point also to those responses.

Green, R. E., Bower, A. S. and Lugo-Fernandez, A.: First Autonomous Bio-Optical Profiling Float in the Gulf of Mexico Reveals Dynamic Biogeochemistry in Deep Waters, PLoS ONE, 9(7), 1–9, doi:10.1371/journal.pone.0101658, 2014.

Martinez-Vicente, V., Dall'Olmo, G., Tarran, G., Boss, E. and Sathyendranath, S.: Optical backscattering is correlated with phytoplankton carbon across the Atlantic Ocean, Geophysical Research Letters, 40, 1154–1158, doi:10.1002/grl.50252, 2013.

Rasse, R., Dall'Olmo, G., Graff, J., Westberry, T. K., van Dongen-Vogels, V. and Behrenfeld, M. J.: Evaluating Optical Proxies of Particulate Organic Carbon across the Surface Atlantic Ocean, Frontiers in Marine Science, 4(November), 1–18, doi:10.3389/fmars.2017.00367, 2017.

p. 7, Line 167: What is the range of the vertical resolution of the ROMS model in the upper 200 meters? This information will be useful for comparison with the 1D model.

Response: The 3D model had 36 terrain-following sigma levels which means that the vertical resolution varies with the bathymetry. The vertical resolution in the 3D model ranges from a few meters near the surface to ~50 m near the depth of 200 m around the 1D site. In the revised manuscript, we added a simple description of 3D model resolution to be compared with the 1D model resolution (P8 Lines 200-202).

We also point to our response to comments by Reviewer #1 under 3.2.

p. 8, Line 187: Since the biogeochemical model functional forms are essential to evaluating the model performance and the parameter optimization results, the biogeochemical model equations should be reproduced in this manuscript or in an appendix, rather than referring the reader to a different paper.

Response: The model code is published and freely available and the model equations, originally published in 2006, have recently been republished in the Appendix of Laurent et al. (2017). The model has been used in well over a dozen publications by our group and by hundreds of other researchers (the model is part of the widely used ROMS distribution). We do not agree that it is necessary or frankly appropriate to republish the same equations which each manuscript. This is also not common for other widely used models. In our revised manuscript, we added a specific reference to the equation in the Appendix of Laurent et al. (2017) (P7 Lines 174).

Laurent, A., K. Fennel, W.-J. Cai, W.-J. Huang, L. Barbero, and R. Wanninkhof (2017), Eutrophication- induced acidification of coastal waters in the northern Gulf of Mexico: Insights into origin and processes from a coupled physical-biogeochemical model, Geophys. Res. Lett., 44, 946–956, doi:10.1002/2016GL071881.

p. 8, Line 199: "Zooplankton and small detritus were assumed to amount to 10% of phytoplankton biomass and the remaining fractions of POC attributed to large detritus." Why is this assumption made? Is this assumption only employed to define the initial condition?

Response: This assumption is also used for the open boundary conditions. For the biological model, the open boundary conditions are usually unavailable. Here we assumed the zooplankton and small detritus accounted for 10% of phytoplankton following Gomez et al., 2018 in which 20% was assumed for a different biological model

in the Gulf of Mexico. We also do some sensitivity tests in the first year (2010) by perturbing this fraction to be 5%, 20%, and 40%. As shown in Figure 1, the choice of this fraction has little impact on the model results, e.g. phytoplankton, zooplankton, and POC. In the revised manuscript, we also added a short comment on this assumption (P8 Lines 188-189).

Gomez, F. A., Lee, S.-K., Liu, Y., Hernandez Jr., F. J., Muller-Karger, F. E., and Lamkin, J. T.: Seasonal patterns in phytoplankton biomass across the northern and deep Gulf of Mexico: a numerical model study, Biogeosciences, 15, 3561–3576, https://doi.org/10.5194/bg-15-3561-2018, 2018

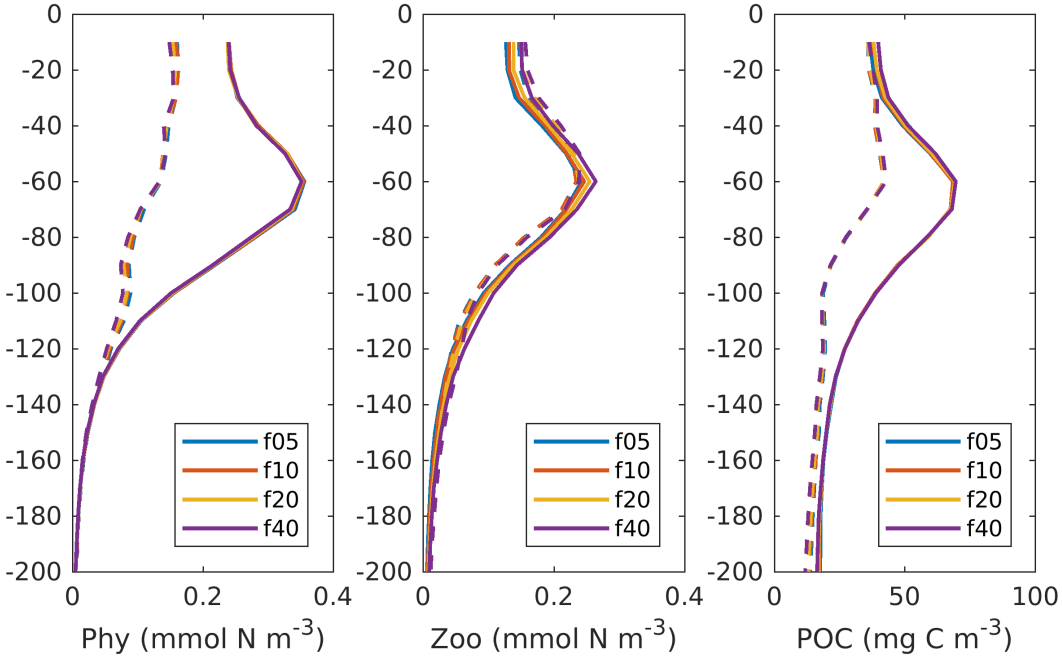

Figure 1. The simulated vertical profiles of phytoplankton, zooplankton, and POC from different sensitivity tests. The solid lines represent median profiles while the dash lines represent interquartile range.

p. 8, Line 210: The 1D model setup is sensible, but more information is needed to understand, evaluate, and reproduce the 1D model - Why is a 5 meter vertical resolution chosen in 1D and is the model sensitive to this choice? - What are the units for the diffusion coefficient and why are these values chosen? They are substantially higher than typical vertical diffusion coefficients in 3D models. - Are all of the parameters that are taken from the 3D model seasonally varying (the mixed layer depth, temperature, solar radiation, and NO3 below 100 meters)? If so, what the temporal frequency at which they are updated? - Why is the temperature and mixed layer depth determined using values from the 3D model rather than the floats, which also have that data?

Response:

There are two main reasons why we chose 5 m. First, the vertical resolution in our BGC-Argo floats is 4-6 meters in the upper 200 m. Second, a 5-m vertical resolution in the 1D model keeps the computational cost reasonable. As stated in sections 3.4 and 3.5 of the manuscript, one parameter optimization experiment ran 36,000 model simulations (30 simulations/generation * 300 generations*4 replications). It took us about one day to run a single

parameter optimization experiment and we performed 13 1D optimization experiments in total (A1-A4, B1-B4, C1-C5). This is in addition to all the 3D model runs we performed.

We are confident the vertical resolution is appropriate because we performed tests of the effect by using different vertical resolutions including 10 m, 5 m, 3 m, and 1 m for optimization C4. As shown in the Figure 2 and 3 below, the choice of vertical resolution has little impact on model results except for some small jumps in the DCM depth (Figure 2e) and DCM magnitude (Figure 2) when the vertical resolution of 10 m is used.

The unit of the diffusion coefficient is m^2 day^{-1} and its value was tuned such that our 1D and 3D models behave similarly.

Finally, the physical input was obtained from daily output of the 3D model. Float data were not used as physical inputs because of their low temporal resolution (~2 weeks).

We added explanations and comments on all of these issues in our revised manuscript (P8 Lines 198-207).

We also point to our responses to comments by Reviewer #1 under 3.2.

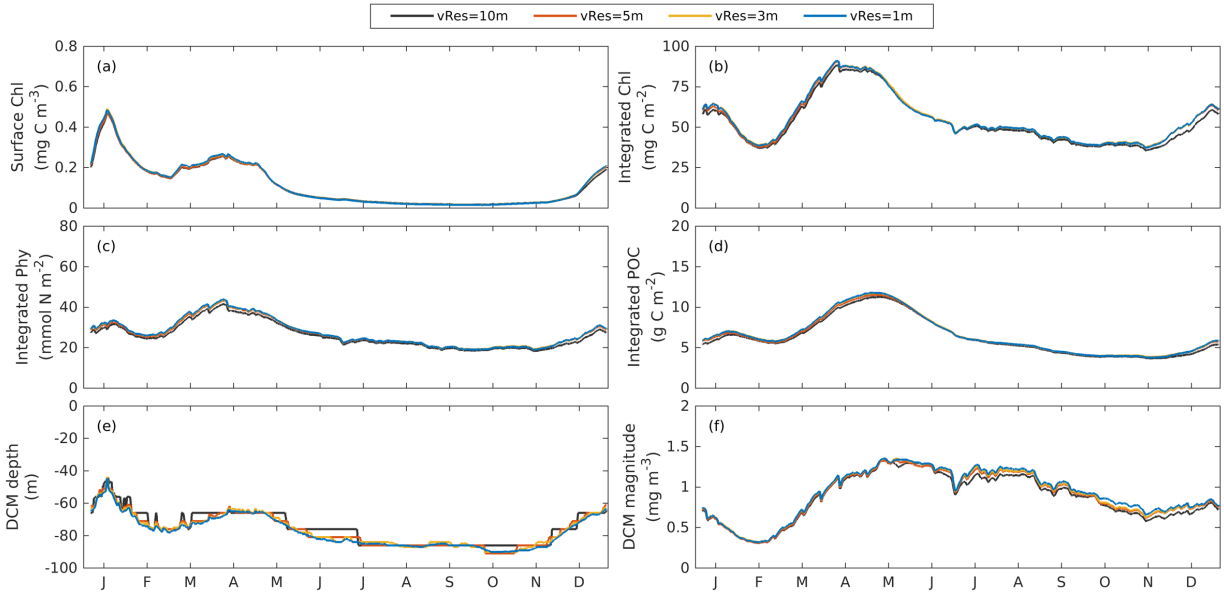

Figure 2. The simulated annual cycle of surface chlorophyll (a),vertically integrated chlorophyll (b), vertically integrated phytoplankton (c), vertically integrated POC(d), and the depth (e) and magnitude (f) of the DCM by using different vertical resolutions.

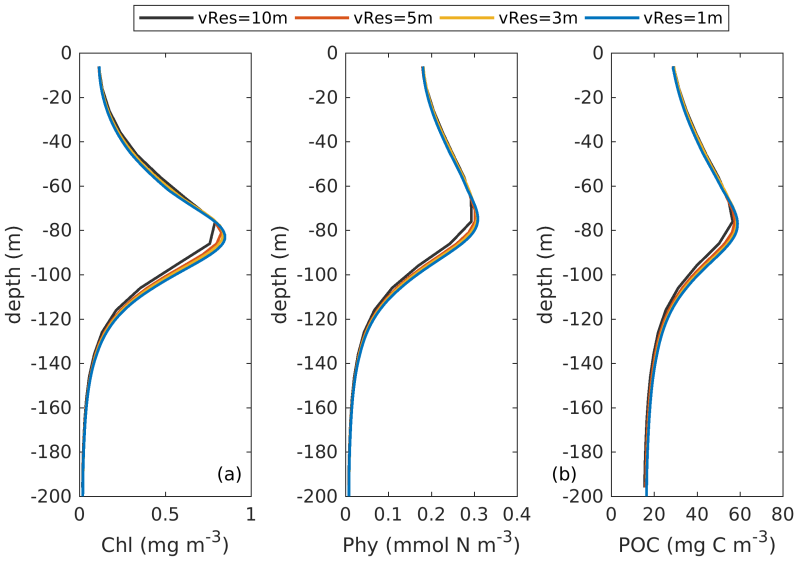

Figure 3. The simulated (colored lines) vertical profiles of chlorophyll, phytoplankton, and POC by using different vertical resolutions.

p. 11, Line 281: Why is the ratio of 0.1 between the sinking speed of the small and large detritus selected? How sensitive are the results to this choice?

Response: We refer to our response to Reviewer #1, comment on Pg 11 line 81-84, which we paste again here for sake of convenience:

These two parameters cannot be constrained simultaneously because they can compensate each other: an increase in the one parameter can be counteracted by a decrease in the other. This is a well-known and much discussed issue in the parameter optimization literature. Basically, there is no information in the available observations that allows to distinguish between the two. Including both parameters in the optimization will degrade the model's predictive skill. To solve this problem, one can either introduce more independent observations or prior knowledge by, e.g. fixing these parameters to their prior values or defining a link between these parameters. Generally, and also in this case, observations are insufficient to constrain all parameters and prior knowledge about the parameters has to be included. This is the common approach to addressing the underdetermination problem of parameter optimization in biological models.

In this study, the ratio of 0.1 was selected based on the prior values of the two parameters. Perturbing and estimating the ratio between two sinking velocities are equivalent to letting both parameters (wSDet and wLDet) into optimization and may degrade model's predictive skills. Without additional information about the depth distribution of Sdet and Ldet, which is not available, the ratio cannot be constrained.

The underdetermination problem and the practice of incorporating prior knowledges is also discussed on P20, L10-28 of our original manuscript.

4. Optimization of 1D model

This section is well written and clear. The discussion of the differences between the surface chlorophyll and vertical profiles is particularly clear and interesting.

Response: Thank you for this comment.

p. 13, Line 329: "Unlike phytoplankton, the observations show that the POC concentrations are 19 mg C m-3 at about 200 m depth because of the existence of detritus (Figure 4c)." What is the evidence that the POC is in the detritus class rather than zooplankton? This point is not supported, but is used later to discriminate between models.

Response: We revised this as follows: *"… the POC concentrations are 19 mg C m-3 at about 200 m depth because of the existence of detritus, or zooplankton, or both"*. We also revised the P15 L70-71 of original manuscript to *"In contrast to the observations where the phytoplankton's contribution is neglectable (Figure 4), the simulated POC at 200 m is dominated by phytoplankton (49%)"*.

Section 4.2: In the section for each experiment, remind the reader what data is used the optimization and which parameters are included in the parameter optimization

Response: As stated already in response to Reviewer 2, we revised as suggested.

Could you plot the mixed layer depth of the 1D model for comparison to the DCM depth? In the 1D model, the mixed layer depth is the main physical control. One option would be to plot the mixed layer depth in figure 3e.

Response: Since the Figure 3e would be busy with a plot of the mixed layer, we plot the seasonal mean levels of the mixed layer in Figure 4 and hope that would convey the information this reviewer was looking for.

The supplemental figure S1 shows that even the corrected satellite data does not capture the seasonality observed by the floats. One sentence here describing the differences that remain between the floats and corrected OC-CCI could help us to better assess why experiment A in particular does not capture the seasonality.

Response: In the experiment A, the satellite estimates of surface chlorophyll was used in parameter optimization and the model results were compared with the satellite data in the Figure 3a. The differences between the satellite and float data would not be a reason for experiment A not capturing the peak of satellite surface chlorophyll. It could be a result of many factors and might be improved by assigning a higher weight on the peaks of surface chlorophyll. However, studying the peaks of surface chlorophyll was not the purpose in this study. Nonetheless, the parameter optimization resulted in a large improvement in surface chlorophyll in the experiment A.

p. 15, Line 375: "Although a slight increase in the misfit occurs for the surface chlorophyll (_5%)," Is the increase of 5% relative to experiment B?

Response: The slight increase here was relative to the base case. The full sentence in the original manuscript is *"Although a slight increase in the misfit occurs for the surface chlorophyll (~5%), the total misfit is reduced by 75% compared to the base case."* We hope this is clear.

Table 2: In the caption, explain what the dashes in the table mean. In the cases where the parameters are not included in the optimization, are the values that are presented in table 1 used? It would be helpful to the reader if the experiment that is discussed in the text is highlighted. Since different parameters are used in the 3D experiment, include additional lines in this table for the parameters that are used in the 3D experiment.

Response: Thanks for this comment. We revised as suggested.

Figure 3: Include what data is used for each experiment in the figure caption. Could error bars be added to the observational points in this figure?

Response: Yes, we revised as suggested.

Figure 4: What do the error bars represent? Are they the interquartile range?
Response: Yes, they are interquartile range. We now state this explicitly in the caption of Figure 4.

5. 3D biogeochemical model
p. 16, Line 421: How were the parameters that were modified manually chosen? It would be useful to provide more discussion of this choice.

Response: Same as comment "5. 3D biogeochemical model" by Reviewer 1 and same response. We paste it again here for sake of convenience:

We did manual modifications because when the resulting parameters were directly applied, the model-data agreement in 3D models was not as well as in 1D models in some aspects, but the most important features were well preserved. In experiment C, chlorophyll concentrations in the upper layer of 3D model were lower than the 1D model and farther away from observations. This might be a result of differences between 1D and 3D models and has been also reported in other studies (e.g. Kane et al., 2011; Hoshiba et al., 2018). However, the depth of the DCM and the non-zero POC concentrations at 200 m with appropriate contributions from each component were well preserved. We therefore did some tests manually by tuning one or two parameters and final set the KNH4 to 0.01 in order to have a better agreement with respect to observations. All of these modifications were based on our tests.

In our case, although the 1D parameter sets could not be used in 3D models directly, they were sufficient to reproduce the main features as in 1D models and largely simplified the following subjective tuning of 3D models by limiting the number of parameters to be adjusted.

We included more explanations for the manual modifications (P16 Lines 400-411) and discussion (P20-21 Lines 522-530) in our revised manuscript.

p. 17, Line 442: Here the authors point to specific parameters that were inappropriate, but on p. 10, Line 246 the authors say that parameters are not allowed to exit a predefined range (which is shown in table 1). This seems inconsistent given that the method could have excluded inconsistent values. Could this difference be explained in more detail?

Response: We think there might be a misunderstanding here. The predefined range of parameters was a collection of their values that had been used in other studies, models, and ecosystem regimes. That means not all parameter values within this range are appropriate for our model. The parameter optimization is therefore to search for an optimal parameter set within this predefined range by minimizing the misfit between model and observations. However, the parameter optimization cannot constrain all parameters (e.g. producing the inappropriate estimates) because of insufficient observations, which is referred to as the underdetermination problem (see earlier responses here and for Reviewer 1). For instance, in our experiment B, the parameter optimization fitted our model to chlorophyll observations but sacrificed other aspects of the model's performance which were degraded, e.g. the vertical profiles of phytoplankton. That is why we said the estimates of the maximum ratio between chlorophyll and phytoplankton (θmax= 0.0158) in experiment B was inappropriate. An appropriate estimate of this parameter requires more independent observations, e.g. of phytoplankton that we used in the experiment C.

Section 5.1: The authors state that the 3D model does not perform well in coastal regions and therefore choose to exclude those regions from the model evaluation. This may be justified based on the statement in section 2 that

there is little cross-shelf exchange in the Gulf of Mexico. However, this point should be discussed in more detail in order to justify ignoring the shelf. In particular, it is important to discuss the extent to which nutrients are supplied to the oligotrophic regions from either the shelf or the open ocean boundary. What is the importance of the boundaries relative to the biogeochemical cycling in the interior? In a 3D model, the boundaries could be very important for setting the primary production in the oligotrophic region.

Response: Firstly, we excluded coastal regions because we have no float data in coastal regions used for parameter optimization and model validation. All parameter optimization experiments in this study were designed for modelling the deep ocean part of the Gulf of Mexico. In our revised manuscript, we clarified this , see P16-17 Lines 419-421.

Secondly, if we define the boundary between coastal regions and open ocean as 1,000 m, the DIN fluxes (NO3+NH4) across the 1,000 m isobath is a sink for the open ocean and nearly balanced by the inputs from open boundaries. Specifically, for the upper 200 m where the primary production occurs, the amount of DIN transported is 2.7×10^{11} mol N yr^{-1} (sink) from the open ocean into coastal region and 2.1×10^{11} mol N yr^{-1} (source) from open boundaries. The primary production in the deep part of the Gulf of Mexico is 10.6×10^{11} mol N yr^{-1} (sink for DIN) which is mainly supported by the vertical transport and interior nitrogen recycle in the upper 200 m.

p. 18, Line 451: What is meant by "different spatio-temporal scales between the two model versions"? This point seems important and could be clarified. Is it referring to time stepping, resolution, retention in a 1D location, or the presence of a seasonal cycle?

Response: The different spatial-temporal scales refer to a lot of factors here. The 1D model is configured in a single station while the 3D model covers the whole Gulf of Mexico. In the vertical direction, the 1D model only simulates the upper 200 m but the 3D model has the whole water column. For temporal scales, the 1D model is simulated for one year but the 3D model runs for 6 years from 2010 to 2016. The model steps are also different between the 1D and 3D models. In our revised manuscript, we removed these sentences but as suggested, we clarified when we talk about the differences between 1D and 3D models (P16 Lines 400-403).

p. 19, Line 479: "cannot" should be "can not"

Response: Revised as suggested.

Assessing the value of BGC Argo profiles versus ocean colour observations for biogeochemical model optimization in the Gulf of Mexico

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Abstract. Biogeochemical ocean models are useful tools but subject to uncertainties arising from simplifications, inaccurate parameterization of processes, and poorly known model parameters. Parameter optimization is a standard method for addressing the latter but typically cannot constrain all biogeochemical parameters because of insufficient observations. Here we assess the trade-offs between satellite observations of ocean colour and biogeochemical (BGC) Argo profiles, and the benefits of combining both observation types, for optimizing biogeochemical parameters in a model of the Gulf of Mexico. A suite of optimization experiments is carried out using different combinations of satellite chlorophyll and profile measurements of chlorophyll, phytoplankton biomass, and particulate organic carbon (POC) from autonomous floats. As parameter optimization in 3D models is computationally expensive, we optimize the parameters in a 1D model version, and then perform 3D simulations using these parameters. We show first that the use of optimal 1D parameters, with a few modifications, improves the skill of the 3D model. Parameters that are only optimized with respect to surface chlorophyll cannot reproduce subsurface distributions of biological fields. Adding profiles of chlorophyll in the parameter optimization yields significant improvements for surface and subsurface chlorophyll but does not accurately capture subsurface phytoplankton and POC distributions because the parameter for the maximum ratio of chlorophyll to phytoplankton carbon is not well constrained in that case. Using all available observations leads to significant improvements of both observed (chlorophyll, phytoplankton, and POC) and unobserved (e.g. primary production) variables. Our results highlight the significant benefits of BGC Argo measurements for biogeochemical parameter optimization and model calibration.

1. Introduction

Oceanic primary production forms the basis of the marine food web and fuels the biological pump, which contributes to the sequestration of atmospheric CO_2 in the ocean's interior thus mitigating global warming. An accurate quantification of primary production and biological carbon export is therefore important for our understanding of the marine carbon cycle and for predicting how carbon cycling and marine ecosystems will interact with climate change.

Direct observations of primary production and export flux are relatively sparse because of the cost and effort involved in measuring these fluxes. Numerical models can complement sparse observations. Well validated and calibrated models are useful tools for hindcasting and nowcasting past and present biogeochemical fluxes and are the most common tool for projecting future changes.

In recent years, many biogeochemical models with different complexities~~, ranging from three to more than thirty biological state variables,~~ have been developed to study ocean biogeochemical processes. Regardless of their complexities, the performance of these models is highly dependent on the appropriate choice of model parameter values (e.g. maximum growth, grazing and mortality rates), most of which are poorly known. ~~Some parameter choices are informed by laboratory experiments (e.g. light and nutrient dependence of phytoplankton growth), although isolated cultures in the lab may not be representative of the behavior of natural communities. Other parameters cannot be directly determined (e.g. mortality rates). Choosing appropriate parameter values becomes more challenging as model complexity grows because the number of parameters increases exponentially with the number of state variables (Denman, 2003).~~ A standard method for choosing these parameters is optimization, a process by which the misfit between model results and available observations is minimized by iteratively varying parameters (Matear, 1995; Prunet et al., 1996a, 1996b; Fennel et al., 2001; Friedrichs et al., 2007; Kuhn et al., 2015, 2018). However, even formal optimization typically cannot constrain all biogeochemical parameters (i.e. provide optimal parameter estimates with relatively small uncertainties) because of insufficient information in the available observations (Matear, 1995; Fennel et al., 2001; Ward et al., 2010; Bagniewski et al., 2011). For example, Matear (1995) used a so-called simulated annealing algorithm to optimize three different ecosystem models and found that even for the simplest nutrient-phytoplankton-zooplankton model, not all independent parameters could be constrained well, leaving the others with large uncertainty ranges. A more recent study reported that the lack of

zooplankton observations led to poor accuracy of the optimized zooplankton-related parameters when using a suite of Lagrangian-based observations during the North Atlantic spring bloom (Bagniewski et al., 2011). A broader suite of observation types should be favourable to parameter optimization although complications can arise. For example, when optimizing a suite of 1D models for the Mid-Atlantic Bight, the use of satellite POC observations in addition to satellite chlorophyll did not yield further improvements in model-data fit but degraded the representation of chlorophyll (Xiao and Friedrichs, 2014a).

Typically surface ocean chlorophyll from satellite is the main source of observations for model validation (e.g. Doney et al., 2009; Gomez et al., 2018; Lehmann et al., 2009) and parameter optimization (Prunet et al., 1996a; Xiao and Friedrichs, 2014a, 2014b), supplemented by other observation types as available. However, satellites only see the ocean surface and do not resolve the vertical distribution of chlorophyll. This is especially problematic in oligotrophic regions where the deep chlorophyll maximum (DCM) is relatively deep and hardly observed by the satellite (Cullen, 2015; Fennel and Boss, 2003). In addition, although chlorophyll has long been used as a proxy of phytoplankton biomass and to estimate primary production based on some assumptions (Behrenfeld and Falkowski, 1997), it is not a direct measure of carbon-based phytoplankton biomass. The ratio of chlorophyll-to-phytoplankton carbon varies by at least an order of magnitude due to physiological responses of phytoplankton to their ambient environment (e.g. nutrients, light, and temperature) (Cullen, 2015; Fennel and Boss, 2003; Geider, 1987). Changes in chlorophyll may result from physiologically induced modifications of the chlorophyll-to-phytoplankton ratio rather than actual changes of phytoplankton biomass (Fommervault et al., 2017; Mignot et al., 2014). Satellite surface chlorophyll alone is therefore likely insufficient for model validation and for constraining biogeochemical models via parameter optimization.

Recent advances in autonomous platforms and sensors have opened opportunities for simultaneous measurement of several biological and chemical properties throughout the upper ocean with high resolution, over broad spatial scales and for sustained periods (Roemmich et al., 2019). In particular, the biogeochemical (BGC) Argo program (Johnson and Claustre, 2016; Roemmich et al., 2019) will provide temporally evolving 3D information on biogeochemical variability at previously unobserved scales. Here we assess to what degree observations of chlorophyll fluorescence and particle backscatter from Argo profiles improve the prospects of optimizing a biogeochemical model for the Gulf of Mexico.

Since the high computational cost and storage demands of 3D models make direct application of most parameter optimization techniques difficult (but see Mattern et al., 2012; Mattern and Edwards, 2017; Tjiputra et al., 2007 for exceptions), they are typically applied in computationally efficient 1D models before using the resulting parameters in 3D version (e.g. Hoshiba et al., 2018; Kane et al., 2011; Kuhn and Fennel, 2019; Schartau and Oschlies, 2003). We follow the latter approach here.

The main objective of this study is to assess the added value of bio-optical profile information from Argo floats for biogeochemical model optimization in the Gulf of Mexico. We first examine the feasibility of improving the 3D model by applying the optimal parameters from 1D model optimizations with some minor manual modifications. We find that the gains from the 1D optimizations transfer to the 3D version. Then, by using different combinations of satellite and float observations we show that parameters optimized with respect to satellite data cannot reproduce subsurface distributions unless the float observations (i.e. chlorophyll, phytoplankton, and POC) are also used.

2. Study region

The Gulf of Mexico (GOM) is a semi-enclosed marginal sea (Figure 1) which is characterized by eutrophic coastal waters on the northern shelf and an oligotrophic deep ocean. The high productivity in the northern coastal region is fueled by large nutrient and freshwater inputs from the Mississippi and Atchafalaya Rivers. The large nutrient load and strong stratification driven by Mississippi and Atchafalaya River inputs lead to summer hypoxia and ocean acidification in bottom waters on the northern shelf (Laurent et al., 2017; Yu et al., 2015), but nutrient export across the shelf break into the open Gulf is minor (Xue et al., 2013).

The deep ocean of the GOM is oligotrophic. Previous satellite-based studies have revealed a clear seasonal cycle in surface chlorophyll with highest concentrations in winter and lowest in summer (Martínez-López and Zavala-Hidalgo, 2009; Muller-Karger et al., 1991, 2015). Thanks to advances in autonomous profiling technology, recent studies based on simultaneous measurements of subsurface chlorophyll and backscatter have demonstrated that the seasonal variability of surface chlorophyll might be a result of the vertical redistribution of subsurface chlorophyll and/or physiological response to solar radiation of phytoplankton (Fommervault et al., 2017; Green et al., 2014).

3. Methods

3.1. Biological observations

Monthly averaged satellite chlorophyll from the Ocean-Colour Climate Change Initiative project (OC-CCI, https://www.oceancolour.org) with a spatial resolution of 4 km from 2010 to 2015 was used for model validation and parameter optimization. These data were provided by the European Space Agency (ESA), which produced a set of validated and error-characterised global ocean-color products by merging SeaWiFS (Sea-viewing Wide Field-of-view Sensor), MODIS (Moderate-resolution Imaging Spectroradiometer), MERIS (medium-spectral resolution imaging spectrometer), and VIIRS (Visible Infrared Imaging Radiometer Suite) products.

In addition to the satellite-based measurements, bio-optical measurements from six autonomous profiling floats were used (Figure 1), which were deployed by the Bureau of Ocean Energy Management (BOEM) and operated in the deep GOM from 2011 to 2015. These floats were equipped with a CTD and bio-optical sensors to collect biweekly profiles of temperature, salinity, chlorophyll, and backscatter at 700 nm (*bbp700* (m^{-1})) from the surface to 1000 m depth (see Fommervault et al., 2017 and Green et al., 2014 for more details). Chlorophyll was derived from fluorescence based on the sensor manufacturer's calibrations and compared with the satellite estimates of surface chlorophyll. While the surface chlorophyll measurements from the floats and the satellite estimates both showed a typical seasonal cycle and were highly correlated (R^2=0.74; see Figures S1 and S2a in the Supplement), the satellite underestimated the float-measured chlorophyll concentrations in winter (Figure S1c). Satellite estimates were therefore corrected following the regression equation shown in Figure S2a.

The backscatter sensor carried by the floats provided the volume scattering function at a centroid angle of 140° and a wave length of 700 nm ($\beta(140^o, 700nm)$ m^{-1} sr^{-1}). The profiles were filtered (Briggs et al., 2011) to remove spikes and then converted into *bbp700* following Green et al. (2014). After that, profiles of *bbp700* were converted into *bbp470* based on a power law (Boss and Haëntjens, 2016) to obtain the phytoplankton (mmol N m^{-3}) and POC (mg C m^{-3}) estimates:

$$bbp(\lambda 1) = \left(\frac{\lambda 1}{\lambda 2}\right)^{-\gamma} bbp(\lambda 2), \quad (1)$$

$$Phy = 30100 \times (bbp470 - 76 \times 10^{-5}) \frac{1}{12 \times 6.625}, \quad (2)$$

$$log10(POC) = 1.22 \times log10(bbp470) + 5.15. \quad (3)$$

where $\lambda 1$ and $\lambda 2$ represented the measured wavelength, and γ was estimated as 0.78 based on the global measurements. The relationships for phytoplankton (Martinez-Vicente et al., 2013; equ. 2) and POC (Rasse et al., 2017; equ. 3) were obtained from a data set for the Atlantic Ocean that covered a wide range of oceanographic regimes from eutrophic to oligotrophic ecosystems. The scale factors of 12 and 6.625 in equ. 2 represented the molecular weight of carbon and the Redfield ratio to convert phytoplankton concentrations from mg C m^{-3} to mmol N m^{-3}. The intercept 76×10^{-5} in equ. 2 represented the background backscatter of nonalgal detritus, which based on Behrenfeld et al. (2005) was the backscatter value when chlorophyll was zero. However, in this study, the most majority (87%) of *bbp470* in the upper 200m was below the intercept and the resulting phytoplankton concentrations were therefore close to zero, which is unrealistic in the Gulf of Mexico. Therefore, the satellite estimate of *bbp670* from OC-CCI was converted into *bbp700* and compared with the float measurements. Compared to surface chlorophyll, surface *bbp700* has a less distinct seasonal cycle (Figure S3). For example, the coefficient of variation, defined as the ratio between standard deviation and mean to show the extend of variability, is much lower for *bbp700* (0.09 and 0.07 for floats and satellite, respectively) than for chlorophyll (0.31 and 0.26 for floats and satellite, respectively). The float *bbp700* is weakly correlated with the satellite estimates (R^2=0.11) and generally lower by a factor of 0.45 than the satellite estimates (Figure S2b). The *bbp700* profiles were therefore multiplied by 2.2 before being converted to *bbp470*. As a result, the mean value of the *bbp470* ($88 \times 10^{-5}\ m^{-1}$) is close to the intercept in equ.2 when chlorophyll went to zero. Furthermore, the resulting concentrations of phytoplankton biomass and POC as well as the ratio of chlorophyll to phytoplankton biomass are reasonable (please see figures 4 and 10). This gave us confidence in our conversion process for float backscatter and our choice of empirical equations relating backscatter to phytoplankton and POC.

3.2. 3D model description

The physical model was configured based on Regional Ocean Modeling System (Haidvogel et al., 2008; ROMS, https://www.myroms.org) for the Gulf of Mexico (Figure 1). The model has a horizontal resolution of 6~7 km and 36 terrain-following sigma layers with refined resolution near the surface and bottom. The model solved the horizontal and vertical advection of tracers using the Multidimensional positive definitive advection transport

algorithm (MPDATA, Smolarkiewicz and Margolin 1998). Horizontal viscosity and diffusivity were parameterized by a Smagorinsky-type formula (Smagorinsky, 1963), and vertical turbulent mixing was calculated by the Mellor-Yamada 2.5-level closure scheme (Mellor and Yamada, 1982). Bottom friction was specified by a logarithmic drag formulation with a bottom roughness of 0.02 m. The model was forced by 3-hourly surface heat and freshwater fluxes, 6-hourly air temperature, sea level pressure and relative humidity, and 10-m winds from the European Centre for Medium-Range Weather Forecast ERA-Interim product with a horizontal resolution of 0.125° (ECMWF reanalysis, https://www.ecmwf.int/en/forecasts/datasets/reanalysis-datasets/era-interim). A bulk parameterization was applied to calculate the surface net heat fluxes and wind stress. The model was one-way nested inside the 1/12° data-assimilative global HYCOM/NCODA (https://www.hycom.org). Tidal constitutes were neglected in the model.

The biogeochemical model used a 7-component model (Fennel et al., 2006) to simulate the nitrogen cycle in the water column. The model described the dynamics of two species of dissolved inorganic nitrogen (nitrate, NO3, and ammonium, NH4), one function of phytoplankton (Phy), chlorophyll (Chl) as a separate state variable which allowed photo-acclimation based on the model of Geider et al. (1997), one function of zooplankton (Zoo), and two pools of detritus (i.e. small suspended detritus, SDeN, and large fast-sinking detritus, LDeN). Water-sediment interactions were simplified by an instantaneous remineralization parameterization, where detritus sinking out of water column immediately resulted in a corresponding influx of ammonium into the bottom layer. Detailed descriptions of the model equations can be found in Fennel et al. (2006) and Laurent et al. (2017). The biological model parameters are listed in Table 1.

The model received freshwater, nutrients (NO3 and NH4) and organic matter inputs from major rivers along the Gulf coast. Freshwater and nutrients from the Mississippi and Atchafalaya rivers were prescribed based on the daily measurements by the US Geological Survey river gauges. River particulate organic nitrogen (PON) was assigned to the small detritus pool and determined as the difference between total Kjeldahl nitrogen and ammonium (Fennel et al., 2011). Other rivers utilized the climatological estimates of freshwater, nutrients, and PON as in Xue et al. (2013).

Initial and open boundary conditions for NO3 were specified by applying an empirical relationship between NO3 and temperature, derived from the World Ocean Atlas (WOA; Figure S4a), that was applied to the temperature

fields from HYCOM/NCODA. Analogously, empirical relationships between chlorophyll and density (Figure S4b), phytoplankton and density (Figure S4c), and POC and density (Figure S4d) were obtained from the median profiles of the bio-optical floats and used to derive initial and boundary conditions for these variables. Zooplankton and small detritus were assumed to amount to 10% of phytoplankton biomass and the remaining fractions of POC attributed to large detritus. Sensitivity tests showed that changing these allocations had little impact on our model results.

A 6-year (5 January 2010 – 31 December 2015) hindcast was performed that included the period of operation of the bio-optical floats. The first year was considered model spin-up and the next five years are discussed.

3.3. 1D model description

As optimizing a 3D biogeochemical model is computationally expensive, it was more practical to perform the optimization using a reduced-order model surrogate. A surrogate can be a coarser resolution model, a simplified model, or a reduced-dimension model. In this study, a 1D model was used to optimize the biological parameters of the 3D model. This approach has been successfully used previously (Hoshiba et al., 2018; Kane et al., 2011; Oschlies and Schartau, 2005).

The 1D model, which is similar to that used by Lagman et al. (2014) and Kuhn et al. (2015), covered the upper 200 m of the ocean with a vertical resolution of 5 m and was configured at one location in the open Gulf (see Figure 1). This relatively fine vertical resolution was used because it was close to that of our BGC-Argo floats (4~6m in upper 200m) and was much higher than the 3D model whose vertical resolution varies from a few meters near the surface to about 50 m near at 200 m depth around the 1D station. In the vertical direction, the water column was divided into two layers: the turbulent surface layer and a quiescent layer below. A higher diffusion coefficient ($K_{Z1} = \max(H_{MLD}^2/400,10)$, in unit of $m^2 \cdot day^{-1}$) was applied in the turbulent surface layer and a lower diffusion coefficient ($K_{Z2} = K_{Z1}/2$) was assigned to the quiescent bottom layer. The interface between these two layers was determined by the mixed layer depth (H_{MLD}, in unit of m), defined as the depth where the temperature was 5°C lower than at the surface, and was obtained from daily outputs of the 3D model. The model was integrated in time using the Crank-Nicolson scheme for vertical turbulent mixing and an implicit time-stepping scheme for the biogeochemical tracers, which were treated identically to the 3D model. Some of the biogeochemical parameterizations required input of temperature and solar radiation, which were also taken from the 3D model. As

the 1D model did not consider horizontal and vertical advection, NO3 below 100 m was nudged to that from the 3D base simulation with a nudging time scale of 20 days. The 1D model was run for the year 2010 repeatedly for three cycles, with the first two were model spin-up and the last annual cycle used to calculate the misfit between model and observations.

3.4. Parameter optimization method

The evolutionary algorithm described by Kuhn et al. (2015, 2018) was used to search for optimal model parameters by minimizing the misfit between model and observations. The misfit was measured by the following cost function:

$$\mathrm{F}(\vec{p}) = \sum_{v=1}^{V} \mathrm{F}_v(\vec{p}), \tag{4}$$

$$\mathrm{F}_v(\vec{p}) = \frac{1}{N_v \sigma_v^2} \sum_{i=1}^{N_v} \left(\hat{y}_{i,v} - y_{i,v}(\vec{p})\right)^2, \tag{5}$$

where $\vec{p}$ represented the parameters vector, V was the number of different observation types, N_v was the number of observations for each variable, $\mathrm{F}_v(\vec{p})$ was the misfit for observation type v measured as the mean-square difference between observations ($\hat{y}$) and corresponding model estimates ($y(\vec{p})$). The cost function $\mathrm{F}_v(\vec{p})$ was normalized by the standard deviation of each variable type (σ_v) in order to remove the effect of different units.

The algorithm is inspired by the rules of natural selection. Following Kuhn et al. (2015), an initial parameter population of 30 parameter vectors was randomly generated within a predefined range of parameters (see Table 1). The model was evaluated for each parameter vector and the resulting cost function was calculated. For this initial generation and each of the following generations, the half of the population with the lower misfit survived into the next generation. The other half was regenerated through a recombination of survivors in a process analogous to genetic crossover. In addition, each newly generated population was subject to random mutations by multiplying the parameter values by a random value between 0 and 2. Parameter values exceeding the predefined range were replaced by their corresponding minimum or maximum limits to avoid unrealistic values. The above procedure was

performed iteratively for 300 generations to reach the minimum of the cost function, which corresponded to the optimal parameter set.

Previous parameter optimization studies have shown that it is difficult to constrain all model parameters even for very simple ecosystem models because the information content of available observations is typically insufficient (Matear, 1995; Fennel et al., 2001; Ward et al., 2010). Here we conducted sensitivity tests to identify the parameters that were most sensitive to the available observations and chose a subset of these to be optimized. In the **base case**, all parameters were at their initial guess values obtained from the previous literature and some initial tuning (Table 1). Then the **test cases** were run multiple times by incrementally changing one parameter at a time to be the minimum, the first, second and third quartile, and the maximum of its corresponding range while setting the other parameters to their initial guess value (Table 1). The sensitivity was measured as the sum of a normalized absolute difference between the base case (y_{Base}) and the test case (y_{Test})

$$Q(y,\vec{p}) = \frac{1}{m}\sum_{i=1}^{m}\frac{1}{n}\sum_{j=1}^{n}\frac{|y_{Base} - y_{Test}|}{y_{Base}} \quad (6)$$

where *m* is the number of parameter increments (here 5) and *n* is the number of base-test pairs consisting of all 1D model grid cells throughout the whole simulation period for all variables to be compared.

Results of the sensitivity analysis are shown in Figure 2, where parameters are ranked by sensitivity with respect to chlorophyll (Figure 2a) and the sum of chlorophyll, phytoplankton, and POC (Figure 2b). POC is the sum of phytoplankton, zooplankton, and small and large detritus.

3.5. Parameter optimization experiments

For the parameter optimization of the 1D model, satellite chlorophyll within a 3×3 pixel (12 km×12 km area) around the 1D station and monthly climatological profiles from the BGC-Argo floats were used. For the climatological profiles, all float profiles in the Gulf were averaged because the deep Gulf of Mexico is homogenous horizontally and only few profiles were available in the immediate vicinity of the 1D station.

To assess the effects of the optimization with respect to the different observation types, we conducted three groups of experiments in which (A) surface satellite chlorophyll only, (B) surface satellite chlorophyll and float

profiles of chlorophyll, and (C) surface satellite chlorophyll and float profiles of chlorophyll, phytoplankton, and POC were used. For each of these three groups, four to five optimizations were conducted starting with the three most sensitive parameters and then adding one more parameter at a time (Table 2) guided by the sensitivity analysis with respect to observed variables they used. Specifically, groups A and B were based on the sensitivity analysis with respect to chlorophyll, while group C was based on sensitivity analysis with respect to the sum of chlorophyll, phytoplankton, and POC. Each optimization was replicated four times. The optimization with smallest model-data misfit within each group was then used. Prior tests have shown that the available observations cannot simultaneously constrain the sinking rates of small and large detritus (w_{SDet} and w_{LDet}) because an increase in one parameter can be counteracted by a decrease in the other. Therefore, a constant ratio of 0.1 between these two parameters (w_{SDet} =0.1×w_{LDet}) was imposed based on their prior values and only one of the two was optimized. In groups A and B, the aggregation parameter $\boldsymbol{\tau}$ was fixed at 0.05 because prior tests generated unreasonably high values for this parameter.

We report two different metrics of misfits for these groups of experiments. The first metric, which we refer to as the case-specific cost function value, is based on the optimized observations in a given experiment and was minimized by the optimization algorithm, i.e.

$$\mathrm{F}_A(\vec{p}) = \mathrm{F}_{SurfCHL}(\vec{p}), \tag{7}$$

$$\mathrm{F}_B(\vec{p}) = \mathrm{F}_{SurfCHL}(\vec{p}) + \mathrm{F}_{CHL}(\vec{p}), \text{~~and~~} \tag{8}$$

$$\mathrm{F}_C(\vec{p}) = \mathrm{F}_{SurfCHL}(\vec{p}) + \mathrm{F}_{CHL}(\vec{p}) + \mathrm{F}_{Phy}(\vec{p}) + \mathrm{F}_{POC}(\vec{p}). \tag{9}$$

However, the models with lower case-specific misfit do not necessarily have better predictive skill in reproducing the unoptimized observations because of the so-called overfitting problem, e.g. the model might be tuned to reproduce optimized observations through wrong mechanisms (Friedrichs et al., 2006). To account for this, a second metric referred to as the total misfit is given by equ. 9. For group C, the second metric is the same as the

case-specific cost function. For groups A and B, the total misfit metric allows us to assess improvements in the model's predictive skill to represent unoptimized fields.

4. Optimization of 1D models

4.1. Observations and base case

To provide context for the evaluation of our optimization experiments, the observations and the base case will be described first. As shown in Figure 3a, the observed surface chlorophyll shows a clear seasonality with the high concentrations in winter and low concentrations in summer. In the base case, the simulated surface chlorophyll fits observations well. Unlike the surface chlorophyll, the observed integrated chlorophyll as well as the phytoplankton and POC over the upper 200 m tend to be more constant with much less seasonality (Figure 3b-d). This has been reported by Fommervault et al. (2017) who attributed the seasonality of surface chlorophyll to the vertical redistributions of subsurface chlorophyll and/or photoacclimation, rather than real changes in biomass.

The DCM is a ubiquitous phenomenon in the oligotrophic regions and can form independently of the biomass maximum (Cullen, 2015; Fennel and Boss, 2003). In this study, we define the DCM depth as where the maximum of subsurface chlorophyll is. Observations detect a predominant DCM at around 60-100m depth throughout the whole year, with a sharp deepening in June and gradual shoaling after July (Figure 3e), reflecting the seasonality of the solar radiation. Unlike the large variability in the depth of the DCM, its magnitude is relatively constant at around 0.62 mg m^{-3} (Figure 3f). In the annually averaged profiles, the observed DCM is located at about 80 m depth with a concentration of 0.52 mg m^{-3} (Figure 4a). The base case succeeds in reproducing the DCM at 65±7m depth. However, it fails to reproduce the deepening of the DCM in June and the simulated annually averaged depth of DCM is shallower by about 15 m than the observed. The simulated magnitude of the DCM is about 2-fold larger than the observed (Figure 3f and Figure 4a) and hence the base case generally overestimates vertically integrated chlorophyll (Figure 3b).

With respect to phytoplankton and POC, the observed maximum concentration occurs at about 60 m depth, which is 20 m above the DCM (Figure 4b-c). The observed vertical distributions of phytoplankton and POC are not well captured by the base case. For example, phytoplankton and POC in the upper layer are overestimated with the model-data discrepancies exceeding the variability of the observations (Figure 4b-c). As a result, the base case yields an overall overestimation of the vertically integrated phytoplankton and POC (Figure 3c-d).

Figure 4b also shows that both observed and simulated phytoplankton approach zero at about 160 m depth. Unlike phytoplankton, the observations show that the POC concentrations are 19 mg C m^{-3} at about 200 m depth because of the existence of detritus, or zooplankton, or both (Figure 4b, c). However, the base case fails to reproduce this non-zero POC concentrations, indicating that the model might be underestimating the carbon export fluxes at 200 m.

4.2. Results of the optimizations

4.2.1. Model-data misfits

The case-specific cost function values and total misfits for the different 1D optimizations are shown in Figure 5. Not surprisingly, all optimizations result in a reduction of the case-specific cost function values. The extent of the reductions depends on the specific subset of parameters that were optimized. However, the total misfits are not reduced in all optimizations. Optimizations A1 and A2 lead to slightly larger total misfits than the base case and optimization B2 leads to a significantly larger total misfit. The smallest total cost function values are achieved in A4, B4, and C4, i.e. in the experiments where a larger subset of parameters was optimized (6 parameters). The optimal parameter sets (A4, B2, and C4), which are selected based on case-specific misfit from these three groups, will be used in subsequent analyses and hereafter are denoted simply as experiment A, experiment B, and experiment C. Further comparisons are presented below to assess the impact of the different combinations of observations.

4.2.2. Experiment A: Satellite chlorophyll only

The optimal parameters (Table 2) from experiment A yield a 58% reduction in the misfit for surface chlorophyll (Figure 5d). However, the vertical structure of chlorophyll deteriorates relative to the base case (Figure 4a) because of inappropriate estimates of the initial slope (α=0.0101; see table 2) and the maximum ratio of chlorophyll to carbon (θ_{max}=0.0191; see table 2). The annually averaged depth of the DCM is lifted up to around 30±10m and the magnitude of DCM strongly decreases (Figure 3a, 4b). Similar to chlorophyll, these deteriorations also manifest in the vertical phytoplankton and POC distributions (Figure 4b-c). As a result, experiment A underestimates vertically integrated chlorophyll, phytoplankton, and POC (Fig. 3b-d).

4.2.3. Experiment B: Satellite chlorophyll and chlorophyll profiles

Due to the addition of observed chlorophyll profiles to the optimization in experiment B, the misfits for surface and subsurface chlorophyll decrease relative to the base case (Figure 5d), but the reduction in the misfit for surface chlorophyll (38%) is smaller than that in experiment A (58%). A straightforward interpretation is that the addition of subsurface observations reduces the model's degrees of freedom to fit one single observation type (surface chlorophyll). The vertical profile of chlorophyll is reproduced better in experiment B than in the base case and experiment A in that the magnitude of the DCM is closer to the observations, although the DCM depth is still too shallow, on average by about 20 m (Figure 4a). The improvement in the vertical chlorophyll structure results in a better model-data fit of vertically integrated chlorophyll (Figure 3b).

Despite the improvements in chlorophyll, the vertical profiles of phytoplankton and POC exhibit a marked deterioration relative to the base case and experiment A (Figure 4b-c) because the parameter optimization underestimates the maximum chlorophyll-to-carbon ratio ($\boldsymbol{\theta_{max}}$ =0.0158; see table 2). Experiment B leads to an overestimation of phytoplankton and POC relative to the base case with misfits roughly 2.7 and 1.6 times larger than those of the base case, respectively (Figure 5d). Although experiment B reproduces the non-zero POC concentrations at about 200 m depth, the proportion of phytoplankton in the POC pool is incorrect. In contrast to the observations where the phytoplankton's contribution is neglectable (Figure 4), the simulated POC at 200 m is dominated by phytoplankton (49%).

4.2.4. Experiment C: All available observations

Incorporating all observations (i.e. surface chlorophyll and profiles of chlorophyll, phytoplankton, and POC) in experiment C improves the model-data misfits for almost all aspects except for surface chlorophyll (Figure 3). Although a slight increase in the misfit occurs for the surface chlorophyll (~5%), the total misfit is reduced by 75% compared to the base case. As shown in Figure 4a, the annually averaged depth of DCM of 80 m coincides with the observed DCM, primarily because experiment C reproduces the deepening of the DCM in summer. The magnitude of the DCM is also decreased relative to the base case but remains higher than the observed. Phytoplankton and POC profiles exhibit only minor deviations from the observations (Figure 4b-c). Importantly, experiment C reproduces the non-zero POC concentrations at 200 m. In contrast to experiment B, phytoplankton

in experiment C drops to zero at about 160 m and POC is dominated by detritus (85%), which is more consistent with the observations.

4.3. Simulated carbon fluxes

Annually averaged carbon fluxes within the upper 200 m are shown for each experiment in Figure 6. The primary production in the base case amounts to 0.78 g C m^{-2} day^{-1}, of which 37% is consumed by zooplankton, and the remaining 63% flows into detritus pools through sloppy feeding, mortality, and aggregation of phytoplankton. As for the production of detritus, contributions from the phytoplankton and zooplankton pools account for 70% and 30%, respectively. Most of the produced detritus is recycled into the nutrient pool fueling recycled primary production, and only a small fraction is removed from the upper layer through gravitational sinking. As a result, carbon export, which is estimated as the sum of sinking fluxes by phytoplankton and detritus, is only 0.00032 g C m^{-2} day^{-1} and accounts for 0.04% of primary production.

Due to the underestimation of phytoplankton in experiment A, primary production is reduced to 0.21 g C m^{-2} day^{-1} in that case. All other fluxes in the top 200 m decrease relative to the base case as well, except for the export flux which increases to about 0.8% of primary production. This relative increase in export is the result of larger sinking rates of phytoplankton and detritus (w_{Phy}=0.95, w_{LDet} =4.97; see table 2) than those used in the base case.

In contrast to experiment A, experiment B yields an increase of primary production relative to the base case. The proportion of the grazing flux to primary production and the contribution of zooplankton to the production of detritus also increase to about 59% and 52%, respectively. Unlike in the other three experiments, carbon export in experiment B is dominated by the sinking of phytoplankton, reflecting its large contribution to POC at 200 m. Although the simulated POC concentration at 200 m is very close to the observations, the relative contributions of phytoplankton, zooplankton, and detritus are problematic and likely do not result in a better estimation of carbon export (in this case 0.3% of primary production).

In experiment C, primary production is 0.30 g C m^{-2} day^{-1} with 24% flowing to zooplankton. The mortality of zooplankton causes a flux of 0.047 g C m^{-2} day^{-1} to detritus, which accounts for 17% of the production of detritus. Finally, about 24% of primary production is removed from the upper 200 m through gravitational sinking. The simulated export ratio of 24% is within the wide range of reported export ratios, from 6% to 43%, at 120 m depth in the Gulf of Mexico (see Table 3 of Hung et al., 2010). Despite the high degree of uncertainty that exists when

estimating export ratios (e.g., the global mean export ratio varies from ~10% (Henson et al., 2012; Lima et al., 2014; Siegel et al., 2014) to ~20% (Henson et al., 2015; Laws et al., 2000)), it is obvious that only experiment C reproduced an export ratio of a reasonable magnitude. A more detailed validation of primary production and export fluxes will be presented in the following sections.

5. 3D biogeochemical model

The optimal parameter sets from the 1D optimizations of A, B, and C were applied in the 3D model for the whole GOM for five years (2011-2015). The performance of the 3D model can be regarded as a cross-validation of the parameters optimized in 1D at different times and locations. It is possible that the optimization algorithm has modified parameters to compensate for biases between 1D and 3D simulations, e.g. the absence of advection in 1D model as well as the differences in the model domain, model period, and model resolution, that degrades the 3D model performance (Kane et al., 2011). Indeed, directly applying the optimal parameter sets from 1D version to the 3D model yields lower model-data agreement than the 1D counterpart but well preserves the most important features. For instance, when the resulting parameters are used in the experiment C, chlorophyll concentrations in the upper layer were lower in the 3D model and farther away from the observations. However, the DCM depth and the non-zero POC concentrations at 200 m with appropriate contributions from each component are well reproduced in the 3D model. We therefore performed a few manual tests and made the following modifications to the optimized parameters to bring the model-data agreement of 3D model in better alignment with that of 1D version (Table 2): the half-saturation for NH_4 uptake (k_{NH4}) was decreased to 0.01 in experiment B and C, and the aggregation parameter (τ) was decreased to 0.05 in the experiment C.

5.1. Spatial patterns of surface chlorophyll

First, the annual climatological surface chlorophyll from satellite and model are compared from 2011 to 2015. The satellite estimates show high chlorophyll in the coastal regions and low chlorophyll in the deep ocean (Figure 7a). This spatial pattern of surface chlorophyll is well reproduced in all simulations except in the experiment A which even fails to reproduce the relatively high chlorophyll near the Mississippi-Atchafalaya river systems because of the high sinking rate of phytoplankton (w_{Phy}=0.95; see Table 2). The largest model-data differences occur in the coastal regions, where all simulations underestimate the observed surface chlorophyll. Since all BGC-Argo floats operated in the deep ocean (Figure 1) and the parameter optimization is performed at one central station

without any influence from coastal environments, only the model results in the deep ocean (depth > 1000 m) will be considered in the following discussion.

5.2. Subsurface distributions

Figure 8 shows the seasonal cycles of surface chlorophyll as well as the vertically integrated chlorophyll, phytoplankton, and POC within the deep ocean (depth>1000 m). Analogous to the 1D models, chlorophyll, phytoplankton, and POC were integrated over the upper 200 m. Here again the whole deep ocean was averaged because it is homogenous horizontally. In addition, we compare surface chlorophyll with satellite estimates in two sub-regions from the Mississippi Delta and the central Gulf in Figure S5.

Comparisons of vertical profiles between observations and model results are given in Figure 9. In general, the main features in the 3D models are very similar to those in 1D. Experiment A cannot constrain the vertical profiles of chlorophyll because of the inappropriate estimation of initial slope (α), experiment B overestimates phytoplankton and its contribution to POC since the maximum ratio of chlorophyll to carbon (θ_{max}) is weakly constrained, and experiment C shows significant improvements in the model-data agreement.

Additional comparisons of the chlorophyll-to-carbon ratio, primary production, and carbon export fluxes from 1D and 3D models with observations are given in Figure 10. The chlorophyll-to-carbon ratio is estimated as the vertically integrated chlorophyll divided by phytoplankton in the upper 200 m (Figure 10a). As an important indicator of phytoplankton physiological status (Geider, 1987), the observed chlorophyll-to-carbon ratio varies considerably in response to the ambient environment. In general, the ratios derived from the 3D models are lower than their corresponding 1D values, but the differences are still within the range of variability. Without utilizing the observations of phytoplankton and POC, experiments A and B in both 1D and 3D versions underestimate the chlorophyll-to-carbon ratio. In experiment C, the simulated chlorophyll-to-carbon ratios from 1D and 3D are in good agreement with the observations although the observed variability is underestimated.

For reference, satellite-based primary production (PP) is provided by two algorithms, the Vertically Generalized Production Model (VGPM, Behrenfeld and Falkowski 1997) and the Carbon-based Productivity Model (CbPM, Westberry et al. 2008). As shown in Figure 10b, satellite-based PP differs depending on the algorithm applied. PP results from all 3D simulations which were integrated down to 200 m are qualitatively similar

to the 1D simulations. Experiment C provides the best estimates of PP when compared to satellite-based estimates from VGPM and CbPM, both in 1D and 3D.

The base case and experiments A and B yield carbon export fluxes smaller by one to two orders of magnitude than experiment C. Thus, only experiment C from the 1D and 3D models are shown in Figure 10c in comparison to observations from sediment traps (see supplementary material). The carbon export fluxes at 200 m from the 1D and 3D are similar in magnitude although the 1D model yields higher fluxes and larger variability. Despite the scarcity of carbon export observations in the GOM, the model estimates are within the range of observations down to ~1,600 m and capture the observed declining trend of carbon export with depth.

In summary, all the results above demonstrate the feasibilities of using the locally optimized parameters from the 1D model to improve the 3D simulation. In addition, by incorporating all available observations (i.e. surface chlorophyll from satellite estimates, profiles of chlorophyll, phytoplankton, and POC from bio-optical floats), experiment C can not only simulate the biogeochemical processes well in the upper 200 m, but also reproduce the carbon export flux and its associated attenuation in the deep ocean (200-1600m) of the GOM.

6. Discussion

6.1. Trade-offs between different observations for parameter optimization

The results of the optimization experiments vary dramatically depending on how many observation types are used. Using only satellite surface chlorophyll in experiment A succeeds in reducing the misfits of surface chlorophyll, but at the expense of the vertical structure since the predominant DCM disappears in experiment A. Satellite surface chlorophyll alone cannot constrain several vital parameters, including the initial slope of the productivity-irradiance curve ($\boldsymbol{\alpha}$) and the maximum ratio of chlorophyll to carbon ($\boldsymbol{\theta_{max}}$), with confidence. This result highlights the importance of subsurface observations for parameter optimization and similarly for model validation.

The floats provide valuable subsurface observations, but chlorophyll profiles alone are not sufficient for parameter optimization. In experiment B, the addition of chlorophyll profiles leads to significant improvements in vertical chlorophyll distributions; however, the profiles of phytoplankton and POC deteriorate largely because the maximum ratio of chlorophyll to carbon ($\boldsymbol{\theta_{max}}$) is poorly constrained. Using estimates of phytoplankton biomass and POC derived from backscatter measurements in experiment C yields the best estimation of plankton-related

state variables and carbon fluxes (i.e. primary production and carbon export). Only in this experiment do the improvements obtained from observations in the upper 200 m extend to the deep ocean as reflected in the improved carbon export estimates below 1,000 m.

It should be noted, however, that degradation of unoptimized variables did not occur in all optimizations within experiments A and B. In some cases, the unoptimized fields were improved. For example, the A2 optimization yields a 69% reduction in the misfit for subsurface chlorophyll (Figure 5d) and large improvements of chlorophyll profiles (Figure S6a) even though no observations of subsurface chlorophyll are used. Another example is that B1 optimization improves simulations of phytoplankton and POC (Figure 5d and Figure S6b-c) through the correlations between the observed chlorophyll and phytoplankton ($R^2 = 0.69$) and POC ($R^2 = 0.69$). Similar findings have been reported in Prunet et al. (1996b) where the improvements of chlorophyll profiles within the mixed layer were obtained by using surface chlorophyll in a 1D model. In a more recent study by Xiao and Friedrichs (2014a) where satellite data was used subsurface fields were improved in addition to surface fields.

In optimizations A2 and B1, the improvement in unoptimized fields occurred because the poorly constrained parameters were not optimized but well defined coincidently ($\boldsymbol{\alpha} = 0.125$ in the optimization A2 and $\boldsymbol{\theta_{max}} = 0.0535$ in the optimization B1; see table 2). Including the poorly constrained parameters into the parameter optimization can return a lower misfit with respect to the observations used in optimization but increases the risk of overfitting and reduces the model's predictive skill, i.e. the ability to simulate unoptimized observations and those collected at different locations and times. This is consistent with previous studies (Friedrichs et al., 2006, 2007; Ward et al., 2010). For example, Friedrichs et al. (2006) optimized three ecosystem models of different complexities against three seasons of observations and the resulting parameters were used to quantify the predictive skill for the fourth season. Cross-validation showed that exclusion of the poorly constrained parameters from the optimization increased the predictive skill.

Although prior knowledge of the parameters allows one to exclude those poorly constrained ones from the optimization and thus can prevent degradation in unoptimized variables, most parameters are poorly known. Thus, the ultimate resolution of this issue should be to increase availability of observations so that more parameters can be constrained with confidence. In addition, even if the poorly constrained parameters are well-known, a lack of observations hampers our ability to recognize improvements in the model's predictive skill and hence may prevent

us from identifying the optimal solutions. For example, without the observations of phytoplankton and POC, we could not have known that optimization B1 improved simulations of phytoplankton and POC, let alone that the optimization B1 was a better solution than the optimization B2 (the experiment B) in terms of the lower total misfit as shown in Figure 5d.

It has been suggested that when performing a parameter optimization, not only parameter values but also parameter uncertainties should be taken into account (Fennel et al., 2001; Ward et al., 2010; Bagniewski et al., 2011). The parameter uncertainties can be assessed by performing an uncertainty analysis (Fennel et al., 2001; Prunet et al., 1996a, 1996b), replicating the parameter optimization (Ward et al., 2010), and cross-validating the resulting parameters (Xiao and Friedrichs, 2014a). In this study, a cross-validation of the parameters was conducted by evaluating the model's predictive skill with respect to different variables, times, and locations. However, even when cross-validation at different times and locations produces large misfits, we cannot conclude that the models reproduce observations through wrong mechanisms. This is because the large misfit can be a result of intrinsic heterogeneity of biological parameters at different times (Mattern et al., 2012) and locations (Kidston et al., 2011). Therefore, it is important to evaluate the predictive skill of unoptimized variables.

Collectively, the discussion above highlights the values of BGC float data for parameter optimization and model validation, not only because of their high spatio-temporal coverage but also their ability to measure multiple properties simultaneously.

6.2. Feasibilities of applying the local optimized parameters to 3D models

As the high computational cost makes direct optimization for a 3D biogeochemical model impractical, we performed parameter optimizations first in a 1D surrogate model with the same biogeochemical component as the 3D model. However, there are some difficulties in porting the locally optimized parameters to the basin-scale model.

Firstly, the 1D model necessarily neglects advection and inevitably differs from the 3D model, e.g. in model domain and model resolution. The optimized parameters from the 1D model may have been adjusted to compensate for biases between 1D and 3D models and, as a result, this may degrade the 3D simulations (Kane et al., 2011). Although counter examples also exist where the 3D simulations outperform the 1D models with respect to vertical profiles of phytoplankton and nitrate (Hoshiba et al., 2018), some manual modifications might be necessary before

the optimal 1D parameters can be applied in the 3D model. In this study, despite some degradations in 3D simulations, the benefits of the 1D optimization were mostly preserved in the 3D simulations. This greatly simplified the following subjective tuning of the 3D model by limiting the number of parameters that needed to be adjusted and confirmed the feasibility of improving the 3D model by optimizing a 1D surrogate.

Secondly, the spatial heterogeneity of parameters (e.g., Kuhn and Fennel 2019) is another issue that influences the portability of parameters from 1D to 3D models. For example, the underestimation of surface chlorophyll in the coastal regions may result from the contrasting ecosystem functioning between coastal regions and deep ocean, whereby the highly productive continental shelf in the northern GOM is fueled by the large nutrient load from the Mississippi and Atchafalaya river systems with primary production being as high as 4 g C m^{-2} day^{-1} near the Mississippi river delta (Fennel et al., 2011), while the deep ocean is oligotrophic and nutrient limited with the primary production ranging from 0.2 to 0.5 g C m^{-2} day^{-1} (see Figure 10). In some studies, the parameter optimization has been performed at several contrasting stations with a goal of using different parameter sets in different regions of the 3D model (Hoshiba et al., 2018). In other studies different stations were optimized simultaneously to obtain one single optimized parameter set (Kane et al., 2011; Oschlies and Schartau, 2005; Schartau and Oschlies, 2003). Such parameters compromise the misfit in each single station but take account into all stations and can often yield an overall better simulation of all these stations as shown by Kuhn and Fennel (2019).

7. Conclusions

In this study, we have performed parameter optimization for a 1D biogeochemical model and then used the resulting parameters with a few modifications to generate simulations with a corresponding 3D model in the GOM. Three experiments have been conducted by using different combinations of observations (surface chlorophyll from satellite estimates, vertical profiles of chlorophyll, phytoplankton biomass and POC from BGC Argo floats) in order to examine the trade-offs between the different observations for parameter optimization. Two misfit metrics have been defined using the case-specific misfit and the total misfit to measure the models' abilities to reproduce the optimized and unoptimized observations.

Model results show that satellite surface chlorophyll alone cannot reproduce well the vertical structures in a biogeochemical model unless profile observations are used in addition. BGC Argo floats are an excellent platform

for obtaining such observations at high spatio-temporal coverage and for a relatively broad suite of parameters. Only adding chlorophyll profiles is not sufficient because they fail to constrain the ratio of chlorophyll to phytoplankton, but the addition of backscatter, which allows estimation of phytoplankton biomass and POC, enables us to constrain the subsurface carbon state variables and reproduce well PP and carbon export fluxes to below1000 m depth. Finally, our 3D model was improved and reproduced similar results as the 1D version, which is promising for the application of parameter optimization.

Code and data availability: The ROMS model code can be accessed at http://www.myroms.com (last access: 16 June 2016). HYCOM data can be downloaded at http://tds.hycom.org/thredds/dodsC/datasets (last access: 16 August 2018). Profiling data from the BGC-Argo floats are available at the National Oceanographic Data Center (NOAA), https://data.nodc.noaa.gov/cgi-bin/iso?id=gov.noaa.nodc:159562 (Hamilton and Leidos, 2017)

Author contributions. BW and KF conceived the study. BW carried out optimization experiments, model simulations and analyses. LY assisted with set-up and validation of the 3D model. CG assisted with processing of the BGC float data. BW and KF discussed the results and wrote the paper with contributions from the coauthors.

Competing interests. The authors declare that they have no conflict of interest.

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References

Bagniewski, W., Fennel, K., Perry, M. J. and D'Asaro, E. A.: Optimizing models of the North Atlantic spring bloom using physical, chemical and bio-optical observations from a Lagrangian float, Biogeosciences, 8, 1291–1307, doi:10.5194/bg-8-1291-2011, 2011.

Behrenfeld, M. J. and Falkowski, P. G.: Photosynthetic rates derived from satellite-based chlorophyll concentration, Limnology and Oceanography, 42(1), 1–20, 1997.

Behrenfeld, M. J., Boss, E., Siegel, D. A. and Shea, D. M.: Carbon-based ocean productivity and phytoplankton physiology from space, Global Biogeochemical Cycles, 19(1), 1–14, doi:10.1029/2004GB002299, 2005.

Biogeochemical-Argo Planning Group: The scientific rationale, design and implementation plan for a Biogeochemical-Argo float array, edited by Ken Johnson and Hervé Claustre., 2016.

Boss, E. B. and Haëntjens, N.: Primer regarding measurements of chlorophyll fluorescence and the backscattering coefficient with WETLabs FLBB on profiling floats., 2016.

Briggs, N., Perry, M. J., Cetinic´, I., Lee, C., D'Asaro, E., Gray, A. M. and Rehm, E.: High-resolution observations of aggregate flux during a sub-polar North Atlantic spring bloom, Deep-Sea Research I, 58, 1031–1039, doi:10.1016/j.dsr.2011.07.007, 2011.

Cullen, J. J.: Subsurface Chlorophyll Maximum Layers : Enduring Enigma or Mystery Solved ?, Annual Review of Marine Science, 7, 207–239, doi:10.1146/annurev-marine-010213-135111, 2015.

Denman, K. L.: Modelling planktonic ecosystems : parameterizing complexity, Progress in Oceanography, 57, 429–452, doi:10.1016/S0079-6611(03)00109-5, 2003.

Doney, S. C., Lima, I., Moore, J. K., Lindsay, K., Behrenfeld, M. J., Westberry, T. K., Mahowald, N., Glover, D. M. and Takahashi, T.: Skill metrics for confronting global upper ocean ecosystem-biogeochemistry models against field and remote sensing data, Journal of Marine Systems, 76, 95–112, doi:10.1016/j.jmarsys.2008.05.015, 2009.

Fennel, K. and Boss, E.: Subsurface maxima of phytoplankton and chlorophyll : Steady-state solutions from a simple model, Limnology and Oceanography, 48(4), 1521–1534, 2003.

Fennel, K., Losch, M., Schroter, J. and Wenzel, M.: Testing a marine ecosystem model : sensitivity analysis and

parameter optimization, Journal of Marine Systems, 28, 45–63, 2001.

Fennel, K., Wilkin, J., Levin, J., Moisan, J., Reilly, J. O. and Haidvogel, D.: Nitrogen cycling in the Middle Atlantic Bight : Results from a three-dimensional model and implications for the North Atlantic nitrogen budget, GLOBAL BIOGEOCHEMICAL CYCLES, 20, 1–14, doi:10.1029/2005GB002456, 2006.

Fennel, K., Hetland, R., Feng, Y. and Dimarco, S.: A coupled physical-biological model of the Northern Gulf of Mexico shelf: Model description, validation and analysis of phytoplankton variability, Biogeosciences, 8, 1881–1899, doi:10.5194/bg-8-1881-2011, 2011.

Fommervault, O. P. De, Perez-brunius, P., Damien, P., Camacho-ibar, V. F. and Sheinbaum, J.: Temporal variability of chlorophyll distribution in the Gulf of Mexico: bio-optical data from profiling floats, Biogeosciences, 14, 5647–5662, doi:10.5194/bg-14-5647-2017, 2017.

Friedrichs, M. A. M., Hood, R. R. and Wiggert, J. D.: Ecosystem model complexity versus physical forcing: Quantification of their relative impact with assimilated Arabian Sea data, Deep-Sea Research Part II, 53, 576–600, doi:10.1016/j.dsr2.2006.01.026, 2006.

Friedrichs, M. A. M., Dusenberry, J. A., Anderson, L. A., Armstrong, R. A., Chai, F., Christian, J. R., Doney, S. C., Dunne, J., Fujii, M., Hood, R., Jr, D. J. M., Moore, J. K., Schartau, M., Spitz, Y. H. and Wiggert, J. D.: Assessment of skill and portability in regional marine biogeochemical models: Role of multiple planktonic groups, Journal of Geophysical Research, 112, 1–22, doi:10.1029/2006JC003852, 2007.

Geider, R. J.: Light and temperature dependence of the carbon to chlorophyll a ratio in microalgae and cyanobacteria: implications for physiology and growth of phytoplankton, New Phytologist, 106, 1–34, 1987.

Geider, R. J., MacIntyre, H. L. and Kana, T. M.: Dynamic model of phytoplankton growth and acclimation : responses of the balanced growth rate and the chlorophyll a : carbon ratio to light , nutrient-limitation and temperature, Marine ecology progress series, 148, 187–200, 1997.

Gomez, F. A., Lee, S., Liu, Y., Jr, F. J. H., Muller-karger, F. E. and Lanmkin, J. T.: Seasonal patterns in phytoplankton biomass across the northern and deep Gulf of Mexico : a numerical model study, Biogeosciencesg, 15, 3561–3576, doi:10.5194/bg-15-3561-2018, 2018.

Green, R. E., Bower, A. S. and Lugo-Fernandez, A.: First Autonomous Bio-Optical Profiling Float in the Gulf of Mexico Reveals Dynamic Biogeochemistry in Deep Waters, PLoS ONE, 9(7), 1–9,

doi:10.1371/journal.pone.0101658, 2014.

Haidvogel, D. B., Arango, H., Budgell, W. P., Cornuelle, B. D., Curchitser, E., Lorenzo, E. Di, Fennel, K., Geyer, W. R., Hermann, A. J., Lanerolle, L., Levin, J., McWilliams, J. C., Miller, A. J., Moore, A. M., Powell, T. M., Shchepetkin, A. F., Sherwood, C. R., Signell, R. P., Warner, J. C. and Wilkin, J.: Ocean forecasting in terrain-following coordinates : Formulation and skill assessment of the Regional Ocean Modeling System, Journal of computational physics, 227, 3595–3624, doi:10.1016/j.jcp.2007.06.016, 2008.

Hamilton, P. and Leidos: Ocean currents, temperatures, and others measured by drifters and profiling floats for the Lagrangian Approach to Study the Gulf of Mexico Deep Circulation project 2011-07 to 2015-06 (NCEI Accession 0159562), Version 1.1, NOAA National Centers for Environmental Information. Dataset, available at https://accession.nodc.noaa.gov/0159562, last access: 25 October 2017.

Henson, S. A., Sanders, R. and Madsen, E.: Global patterns in efficiency of particulate organic carbon export and transfer to the deep ocean, Global Biogeochemical Cycles, 26(1), doi:10.1029/2011GB004099, 2012.

Henson, S. A., Yool, A. and Sanders, R.: Variability in efficiency of particulate organic carbon export: A model study, Global Biogeochemical Cycles, 29(1), 33–45, doi:10.1002/2014GB004965, 2015.

Hoshiba, Y., Hirata, T., Shigemitsu, M., Nakano, H., Hashioka, T., Masuda, Y. and Yamanaka, Y.: Biological data assimilation for parameter estimation of a phytoplankton functional type model for the western North Pacific, Ocean Science, 14, 371–386, doi:10.5194/os-14-371-2018, 2018.

Hung, C.-C., Xu, C., Santschi, P. H., Zhang, S.-J., Schwehr, K. A., Quigg, A., Guo, L., Gong, G.-C., Pinckney, J. L., Long, R. A. and Wei, C.-L.: Comparative evaluation of sediment trap and 234Th-derived POC fluxes from the upper oligotrophic waters of the Gulf of Mexico and the subtropical northwestern Pacific Ocean, Marine Chemistry, 121(1), 132–144, doi:https://doi.org/10.1016/j.marchem.2010.03.011, 2010.

Kane, A., Moulin, C., Thiria, S., Bopp, L., Berrada, M., Tagliabue, A., Crépon, M., Aumont, O. and Badran, F.: Improving the parameters of a global ocean biogeochemical model via variational assimilation of in situ data at five time series stations, Journal of Geophysical Research: Oceans, 116, 1–14, doi:10.1029/2009JC006005, 2011.

Kidston, M., Matear, R. and Baird, M. E.: Parameter optimisation of a marine ecosystem model at two contrasting stations in the Sub-Antarctic Zone, Deep-Sea Research II, 58, 2301–2315, doi:10.1016/j.dsr2.2011.05.018,

2011.

Kuhn, A. M. and Fennel, K.: Evaluating ecosystem model complexity for the northwest North Atlantic through surrogate-based optimization, Ocean Modelling, 142, 101437, doi:https://doi.org/10.1016/j.ocemod.2019.101437, 2019.

Kuhn, A. M., Fennel, K. and Mattern, J. P.: Progress in Oceanography Model investigations of the North Atlantic spring bloom initiation, Progress in Oceanography, 138, 176–193, doi:10.1016/j.pocean.2015.07.004, 2015.

Kuhn, A. M., Fennel, K. and Berman-frank, I.: Modelling the biogeochemical effects of heterotrophic and autotrophic N2 fixation in the Gulf of Aqaba (Israel), Red Sea, Biogeosciences, 15, 7379–7401, doi:10.5194/bg-15-7379-2018, 2018.

Lagman, K. B., Fennel, K., Thompson, K. R. and Bianucci, L.: Assessing the utility of frequency dependent nudging for reducing biases in biogeochemical models, Ocean Modelling, 81, 25–35, doi:https://doi.org/10.1016/j.ocemod.2014.06.006, 2014.

Laurent, A., Fennel, K., Cai, W. J., Huang, W. J., Barbero, L. and Wanninkhof, R.: Eutrophication-induced acidification of coastal waters in the northern Gulf of Mexico: Insights into origin and processes from a coupled physical-biogeochemical model, Geophysical Research Letters, 44(2), 946–956, doi:10.1002/2016GL071881, 2017.

Laws, E. A., Falkowski, P. G., Smith Jr., W. O., Ducklow, H. and McCarthy, J. J.: Temperature effects on export production in the open ocean, Global Biogeochemical Cycles, 14(4), 1231–1246, doi:10.1029/1999GB001229, 2000.

Lehmann, M. K., Fennel, K. and He, R.: Statistical validation of a 3-D bio-physical model of the western North Atlantic, Biogeosciences, 6(10), 1961–1974, doi:10.5194/bg-6-1961-2009, 2009.

Lima, I. D., Lam, P. J. and Doney, S. C.: Dynamics of particulate organic carbon flux in a global ocean model, Biogeosciences, 11(4), 1177–1198, doi:10.5194/bg-11-1177-2014, 2014.

Martínez-López, B. and Zavala-Hidalgo, J.: Seasonal and interannual variability of cross-shelf transports of chlorophyll in the Gulf of Mexico, Journal of Marine Systems, 77, 1–20, doi:10.1016/j.jmarsys.2008.10.002, 2009.

Martinez-Vicente, V., Dall'Olmo, G., Tarran, G., Boss, E. and Sathyendranath, S.: Optical backscattering is

correlated with phytoplankton carbon across the Atlantic Ocean, Geophysical Research Letters, 40, 1154–1158, doi:10.1002/grl.50252, 2013.

Matear, R. J.: Parameter optimization and analysis of ecosystem models using simulated annealing : A case study at Station P, Journal of Marine Research, 53, 571–607, 1995.

Mattern, J. P. and Edwards, C. A.: Simple parameter estimation for complex models — Testing evolutionary techniques on 3-dimensional biogeochemical ocean models, Journal of Marine Systems, 165, 139–152, doi:10.1016/j.jmarsys.2016.10.012, 2017.

Mattern, J. P., Fennel, K. and Dowd, M.: Estimating time-dependent parameters for a biological ocean model using an emulator approach, Journal of Marine Systems, 96–97, 32–47, doi:https://doi.org/10.1016/j.jmarsys.2012.01.015, 2012.

Mellor, G. L. and Yamada, T.: Development of a turbulence closure model for geophysical fluid problems, Reviews of Geophysics and Space Physics, 20(4), 851–875, doi:10.1029/RG020i004p00851, 1982.

Mignot, A., Claustre, H., Uitz, J., Poteau, A., D'Ortenzio, F. and Xing, X.: Understanding the seasonal dynamics of phytoplankton biomass and the deep chlorophyll maximum in oligotrophic environments: A Bio-Argo float investigation, Global Biogeochemical Cycles, 28(8), 1–21, doi:10.1002/2013GB004781, 2014.

Muller-Karger, F. E., Walsh, J. J., Evans, R. H. and Meyers, M. B.: On the Seasonal Phytoplankton Concentration and Sea Surface Temperature Cycles of the Gulf of Mexico as Determined by Satellites, Journal of Geophysical Research, 96, 12645–12665, 1991.

Muller-Karger, F. E., Smith, J. P., Werner, S., Chen, R., Roffer, M., Liu, Y., Muhling, B., Lindo-atichati, D., Lamkin, J., Cerdeira-estrada, S. and Enfield, D. B.: Natural variability of surface oceanographic conditions in the offshore Gulf of Mexico, Progress in Oceanography, 134, 54–76, doi:10.1016/j.pocean.2014.12.007, 2015.

Oschlies, A. and Schartau, M.: Basin-scale performance of a locally optimized marine ecosystem model, Journal of Marine Research, 63(2), 335–358, 2005.

Prunet, P., Minster, J., Ruiz-Pino, D. and Dadou, I.: Assimilation of surface data in a one-dimensional physical-biogeochemical model of the surface ocean 1 . Method and preliminary results, GLOBAL BIOGEOCHEMICAL CYCLES, 10(1), 111–138, 1996a.

Prunet, P., Minster, J., Echevin, V. and Dadou, I.: Assimilation of surface data in a one-dimensional physical-

biogeochemical model of the surface ocean 2. Ajusting a simple trophic model to chlorophyll, temperature, nitrate, and pCO2 data, GLOBAL BIOGEOCHEMICAL CYCLES, 10(1), 139–158, 1996b.

Rasse, R., Dall'Olmo, G., Graff, J., Westberry, T. K., van Dongen-Vogels, V. and Behrenfeld, M. J.: Evaluating Optical Proxies of Particulate Organic Carbon across the Surface Atlantic Ocean, Frontiers in Marine Science, 4(November), 1–18, doi:10.3389/fmars.2017.00367, 2017.

Roemmich, D., Alford, M. H., Claustre, H., Johnson, K., King, B., Moum, J., Oke, P., Owens, W. B., Pouliquen, S., Purkey, S., Scanderbeg, M., Suga, T., Wijffels, S., Zilberman, N., Bakker, D., Baringer, M., Belbeoch, M., Bittig, H. C., Boss, E., Calil, P., Carse, F., Carval, T., Chai, F., Conchubhair, D. Ó., D'Ortenzio, F., Dall'Olmo, G., Desbruyeres, D., Fennel, K., Fer, I., Ferrari, R., Forget, G., Freeland, H., Fujiki, T., Gehlen, M., Greenan, B., Hallberg, R., Hibiya, T., Hosoda, S., Jayne, S., Jochum, M., Johnson, G. C., Kang, K., Kolodziejczyk, N., Körtzinger, A., Traon, P.-Y. Le, Lenn, Y.-D., Maze, G., Mork, K. A., Morris, T., Nagai, T., Nash, J., Garabato, A. N., Olsen, A., Pattabhi, R. R., Prakash, S., Riser, S., Schmechtig, C., Schmid, C., Shroyer, E., Sterl, A., Sutton, P., Talley, L., Tanhua, T., Thierry, V., Thomalla, S., Toole, J., Troisi, A., Trull, T. W., Turton, J., Velez-Belchi, P. J., Walczowski, W., Wang, H., Wanninkhof, R., Waterhouse, A. F., Waterman, S., Watson, A., Wilson, C., Wong, A. P. S., Xu, J. and Yasuda, I.: On the Future of Argo: A Global, Full-Depth, Multi-Disciplinary Array, Frontiers in Marine Science, 6, 439 [online] Available from: https://www.frontiersin.org/article/10.3389/fmars.2019.00439, 2019.

Schartau, M. and Oschlies, A.: Simultaneous data-based optimization of a 1D-ecosystem model at three locations in the North Atlantic : Part I — Method and parameter estimates, Journal of Marine Research, 61, 765–793, 2003.

Shchepetkin, A. F. and Mcwilliams, J. C.: The regional oceanic modeling system (ROMS): a split-explicit, free-surface, topography-following-coordinate oceanic model, Ocean Modelling, 9, 347–404, doi:10.1016/j.ocemod.2004.08.002, 2005.

Siegel, D. A., Buesseler, K. O., Doney, S. C., Sailley, S. F., Behrenfeld, M. J. and Boyd, P. W.: Global assessment of ocean carbon export by combining satellite observations and food-web models, Global Biogeochemical Cycles, 28(3), 181–196, doi:10.1002/2013GB004743, 2014.

Smagorinsky, J.: General circulation experiments with the primitive equations: I. the basic experiment, Monthly

Weather Review, 91(3), 99–164, 1963.

Smolarkiewicz, P. K. and Margolin, L. G.: MPDATA : A Finite-Difference Solver for Geophysical Flows, Journal of computational physics, 140, 459–480, 1998.

Tjiputra, J. F., Polzin, D. and Winguth, A. M. E.: Assimilation of seasonal chlorophyll and nutrient data into an adjoint three-dimensional ocean carbon cycle model : Sensitivity analysis and ecosystem parameter optimization, Global Biogeochemical Cycles, 21, 1–13, doi:10.1029/2006GB002745, 2007.

Ward, B. A., Friedrichs, M. A. M., Anderson, T. R. and Oschlies, A.: Parameter optimisation techniques and the problem of underdetermination in marine biogeochemical models, Journal of Marine Systems, 81, 34–43, doi:10.1016/j.jmarsys.2009.12.005, 2010.

Westberry, T., Behrenfeld, M. J., Siegel, D. A. and Boss, E.: Carbon-based primary productivity modeling with vertically resolved photoacclimation, GLOBAL BIOGEOCHEMICAL CYCLES, 22, 1–18, doi:10.1029/2007GB003078, 2008.

Xiao, Y. and Friedrichs, M. A. M.: The assimilation of satellite-derived data into a one-dimensional lower trophic level marine ecosystem model, Journal of Geophysical Research: Oceans, 119, 2691–2712, doi:10.1002/2013JC009433.Received, 2014a.

Xiao, Y. and Friedrichs, M. A. M.: Using biogeochemical data assimilation to assess the relative skill of multiple ecosystem models in the Mid-Atlantic Bight : effects of increasing the complexity of the planktonic food web, Biogeosciences, 11, 3015–3030, doi:10.5194/bg-11-3015-2014, 2014b.

Xue, Z., He, R., Fennel, K., Cai, W., Lohrenz, S. and Hopkinson, C.: Modeling ocean circulation and biogeochemical variability in the Gulf of Mexico, Biogeosciences, 10, 7219–7234, doi:10.5194/bg-10-7219-2013, 2013.

Yu, L., Fennel, K. and Laurent, A.: A modeling study of physical controls on hypoxia generation in the northern Gulf of Mexico, Journal of Geophysical Research: Oceans, 120(7), 5019–5039, doi:10.1002/2014JC010634, 2015.

Table list

Table 1. Initial values and ranges of primary parameters used in the biogeochemical model

Descriptions (unit)	Symbol	Value	Range
Radiation threshold for nitrification (W m^{-2})	I_0	0.0095[a]	0.005[b]-0.01[b]
Half-saturation radiation for nitrification (W m^{-2})	k_I	0.1[a]	0.01[b]-0.5[b]
Maximum nitrification rate (day^{-1})	n_{max}	0.2[c]	0.01[b]-0.35[b]
Phytoplankton growth at 0 ºC (Dimensionless)	μ_0	0.69[a]	0.1[b]-3.0[b]
Initial slope of P-I curve (mg_C (mg_Chl W m^{-2} $day)^{-1}$)	α	0.125[a]	0.007[a]-0.13[a]
Half-saturation for NO_3 uptake (mmol_N m^{-3})	k_{NO3}	0.5[a]	0.007[a]-1.5[a]
Half-saturation for NH_4 uptake (mmol_N m^{-3})	k_{NH4}	0.5[a]	0.007[a]-1.5[a]
Phytoplankton mortality (day^{-1})	m_P	0.075	0.01[b]-0.2[b]
Aggregation parameter (day^{-1})	τ	0.1	0.01[b]-25[b]
Maximum chlorophyll to carbon ratio (mg_Chl mg_C^{-1})	θ_{max}	0.0535[c]	0.005[a]-0.15[b]
Phytoplankton sinking velocity (m day^{-1})	w_{Phy}	0.1[a]	0.009[a]-25[a]
Maximum grazing rate (day^{-1})	g_{max}	0.6[a]	0.1[b]-4[b]

Half-saturation for phytoplankton ingestion ((mmol_N m^{-3})^2)	k_P	0.5	0.01[b]-3.5[a]
Zooplankton assimilation efficiency (Dimensionless)	β	0.75[a]	0.25[b]-0.75[b]
Zooplankton basal metabolism (day^{-1})	l_{BM}	0.01	0.01[b]-0.15[b]
Zooplankton specific excretion (day^{-1})	l_E	0.1[a]	0.05[b]-0.35[b]
Zooplankton mortality (day^{-1})	m_Z	0.2	0.02[b]-0.35[b]
Small detritus remineralization (day^{-1})	r_{SD}	0.3[c]	0.005[b]-0.25[a]
Large detritus remineralization (day^{-1})	r_{LD}	0.1	0.005[b]-0.25[a]
Small detritus sinking velocity (m day^{-1})	w_{SDet}	0.1[a]	0.009[a]-25[a]
Large detritus sinking velocity (m day^{-1})	w_{LDet}	1[a]	0.009[a]-25[a]

a Fennel et al. (2006); b Kuhn et al. (2018); c Yu et al. (2015)

Table 2. The best fit of parameter set for each optimization experiment. Dashed lines represent these parameters are not included in the parameter optimization and use their prior values. The optimal optimization A4, B2, and C4 which are further discussed and are denoted simply as experiment A, B, and C are highlighted as **bold**.

		w_{Phy}	m_P	k_{NH4}	τ	θ_{max}	α	w_{LDet}
1D model	Base	0.1000	0.0750	0.5000	0.1000	0.0535	0.1250	1.000
	A1	0.0608	0.0100	1.5000	--	--	--	--
	A2	0.6863	0.0100	0.0195	--	0.0169	--	--
	A3	1.6567	0.1978	0.1004	--	0.0250	0.0219	--
	A4	**0.9468**	**0.0737**	**0.2454**	**--**	**0.0191**	**0.0101**	**4.9694**
3D model	A	0.9468	0.0737	0.0100	--	0.0191	0.0101	4.9694
1D model	B1	0.2863	0.0983	1.5000	--	--	--	--
	B2	**0.4217**	**0.0130**	**0.0300**	**--**	**0.0158**	**--**	**--**
	B3	2.1016	0.0176	1.5000	--	0.0346	0.0079	--
	B4	0.0090	0.0100	1.5000	--	0.0361	0.0405	8.3514
3D model	B	0.4217	0.0130	0.0100	--	0.0158	--	--

		w_{Phy}	r_{LD}	m_P	τ	k_{NH4}	w_{LDet}	θ_{max}
1D model	Base	0.1000	0.1000	0.0750	0.1000	0.5000	1.0000	0.0535
	C1	1.9231	0.2500	0.1805	--	--	--	--
	C2	0.9755	0.2500	0.0100	1.1402	--	--	--
	C3	0.4071	0.0630	0.0100	1.8531	0.0070	--	--
	C4	**0.0090**	**0.0050**	**0.0634**	**0.0995**	**0.0431**	**5.6623**	**--**
	C5	0.0090	0.2245	0.0100	0.6451	1.5000	2.5202	0.0614
3D model	C	0.0090	0.0050	0.0634	0.0500	0.0100	5.6623	--

Figure captions

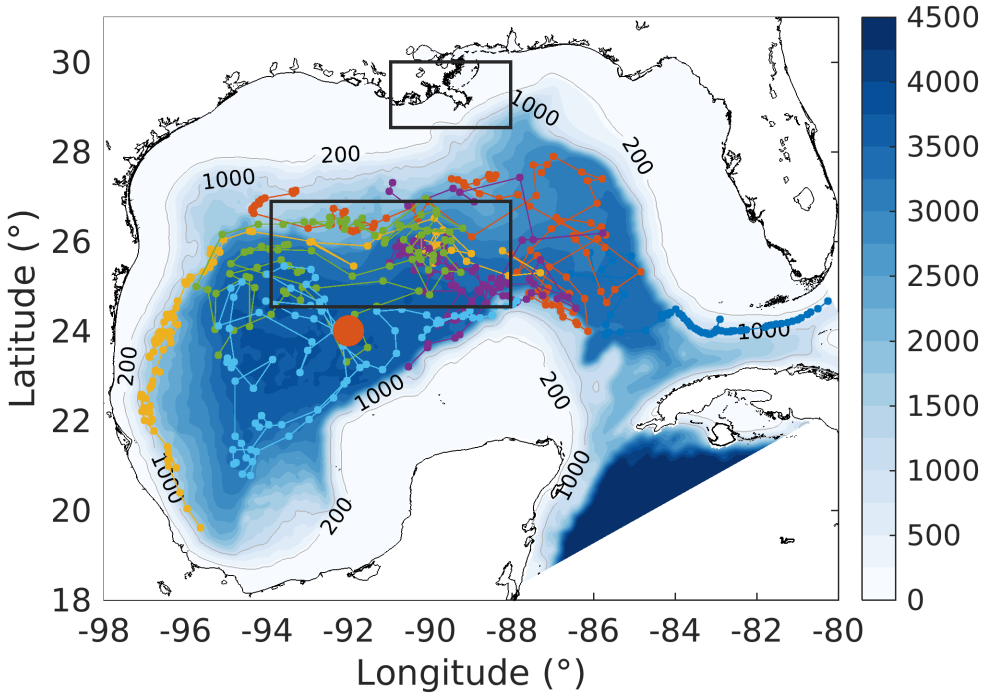


Figure 1. Model bathymetry (unit: m) with trajectories of six bio-optical floats (small colored dots and lines) which were operated in the Gulf of Mexico from 2011 to 2015. The location of the 1D model is denoted by the large orange dot. The north and south black boxes represent the Mississippi Delta and the central gulf, respectively to show comparisons of surface chlorophyll in Figure S5.

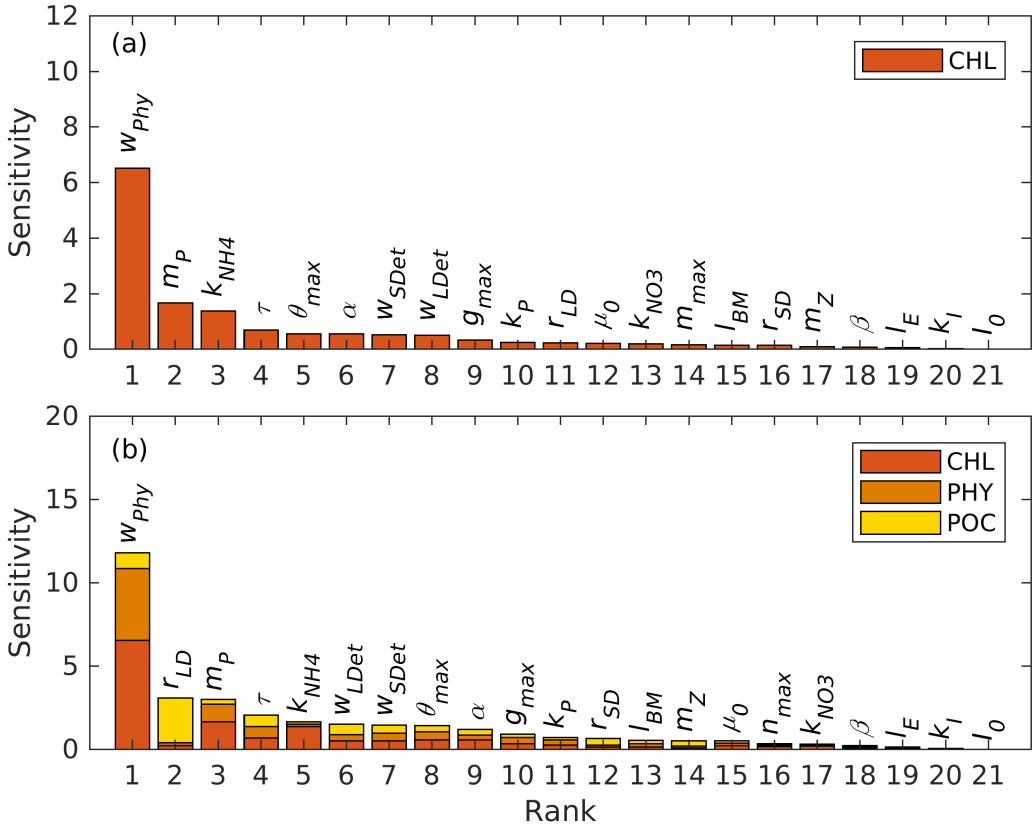
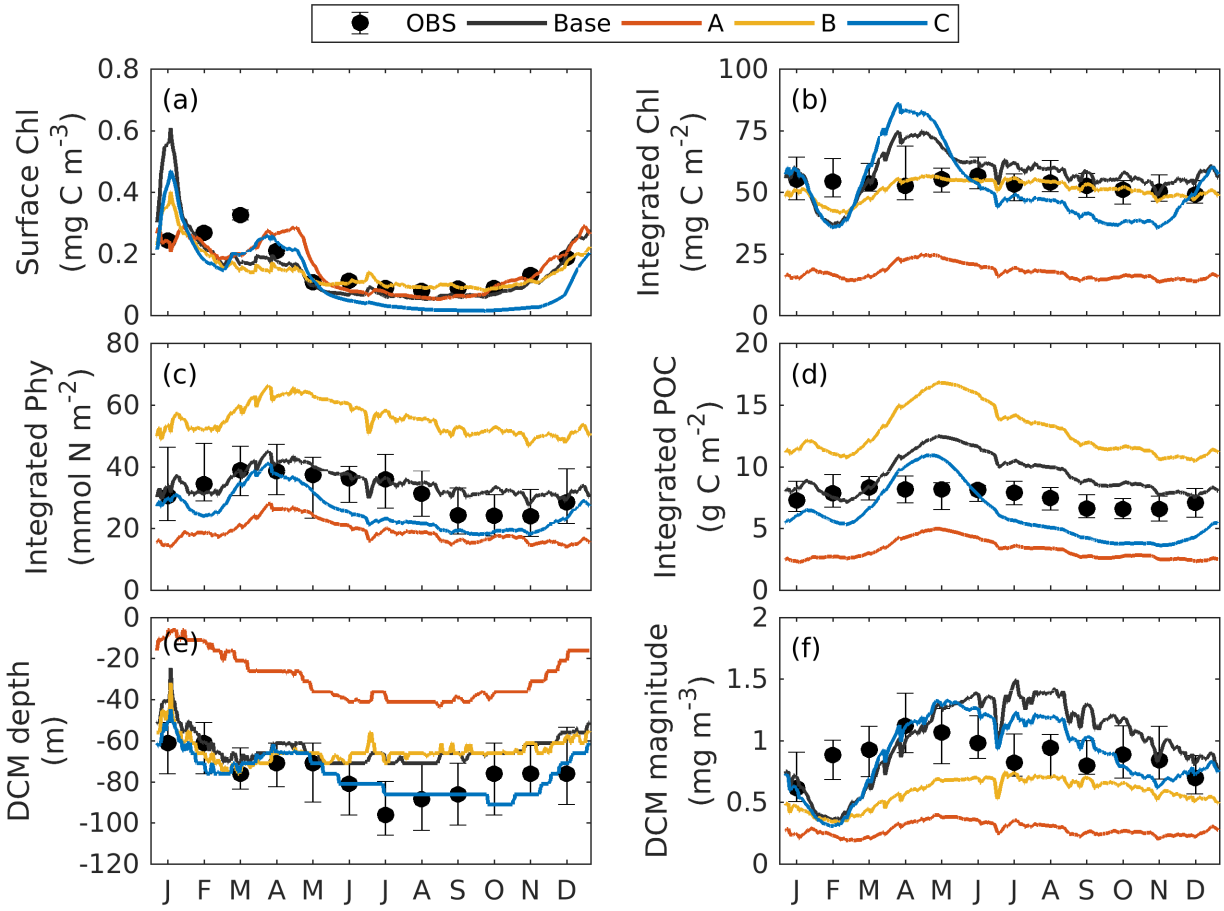


Figure 2. Parameter sensitivities (unit: dimensionless) with respect to (a) chlorophyll and (b) the sum of chlorophyll, phytoplankton, and POC.



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10 Figure 3. Annual cycle of surface chlorophyll (a), vertically integrated chlorophyll (b), vertically integrated
11 phytoplankton (c), vertically integrated POC (d), and the depth (e) and magnitude (f) of the DCM from observations
12 (black dots with error bars), the Base case (black lines), the experiment A (orange lines; only satellite surface
13 chlorophyll is used), B (yellow lines; satellite surface chlorophyll and float profiles of chlorophyll are used), and
14 C (blue lines; all available observations are used). Chlorophyll, phytoplankton, and POC are integrated over the
15 top 200 m. Black error bars represent the interquartile range of observations.

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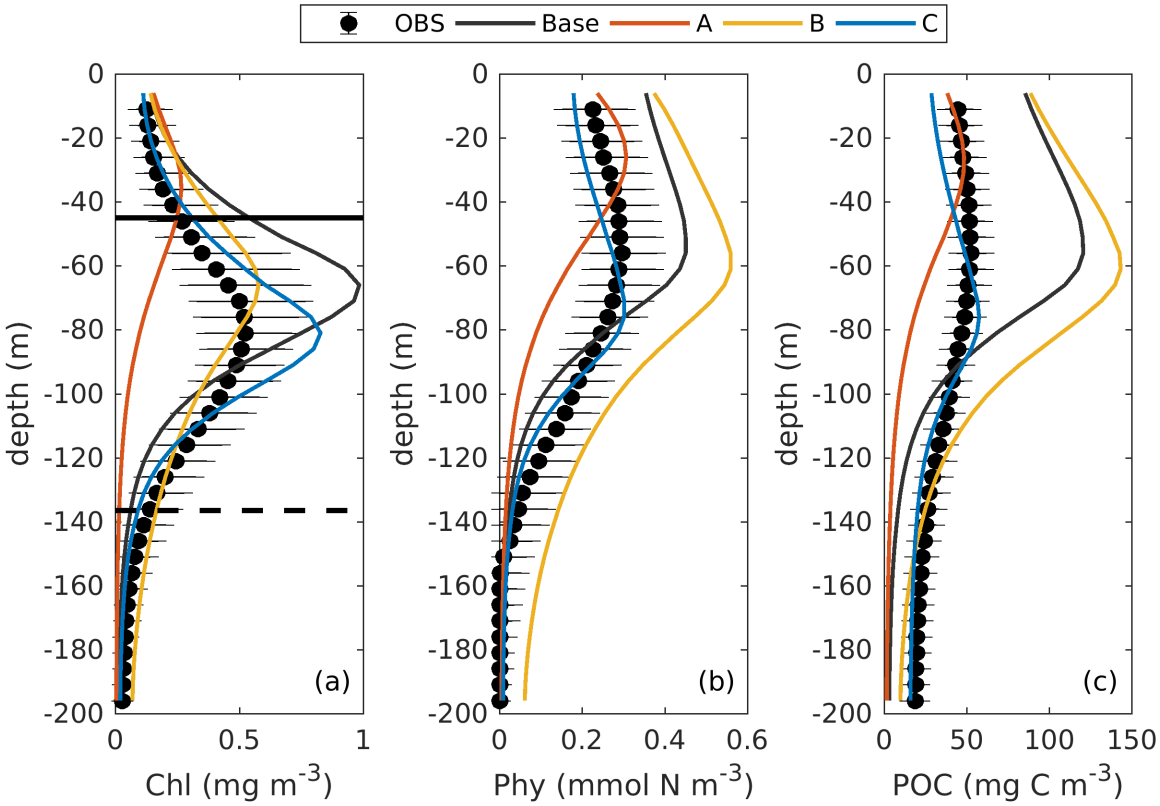

Figure 4. Observed (black dots with error bars) and simulated (colored lines) vertical profiles of chlorophyll, phytoplankton, and POC. Black errors represent the interquartile range of observations. The solid and dashed black lines in panel a represent the median values of mixed layer depth from July and December.

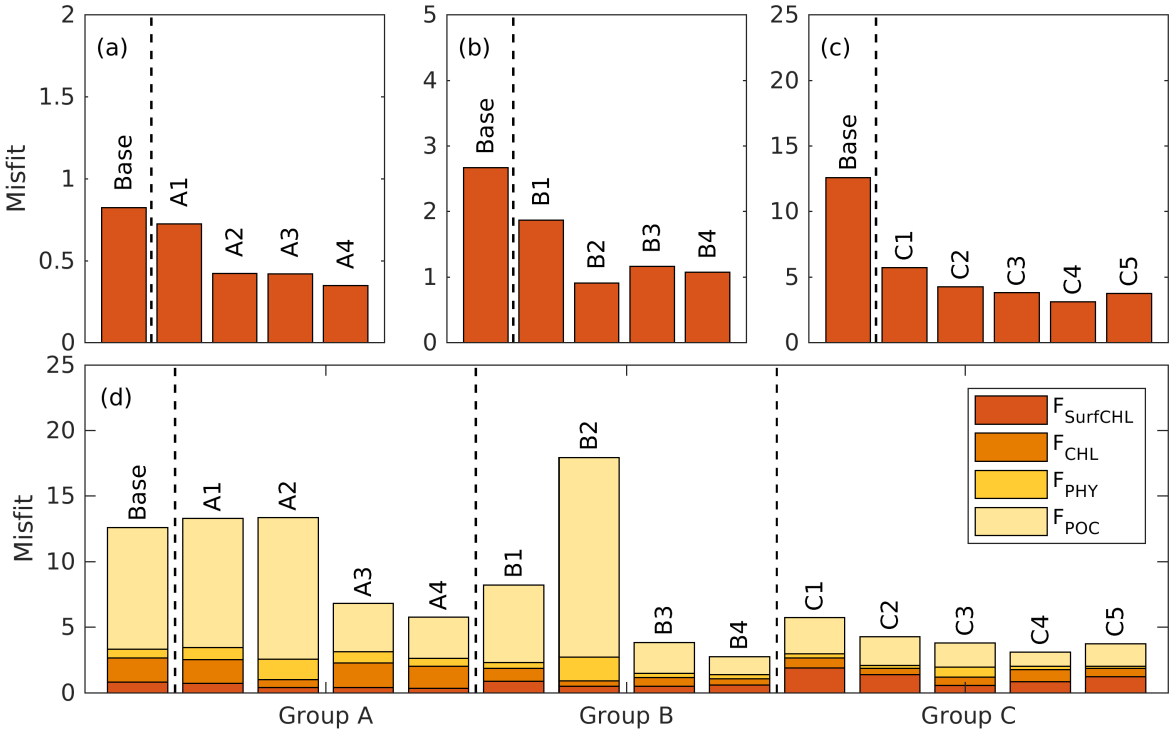

Figure 5. The case-specific cost function values (a-c) and total misfits (d) of the base case and the different optimizations.

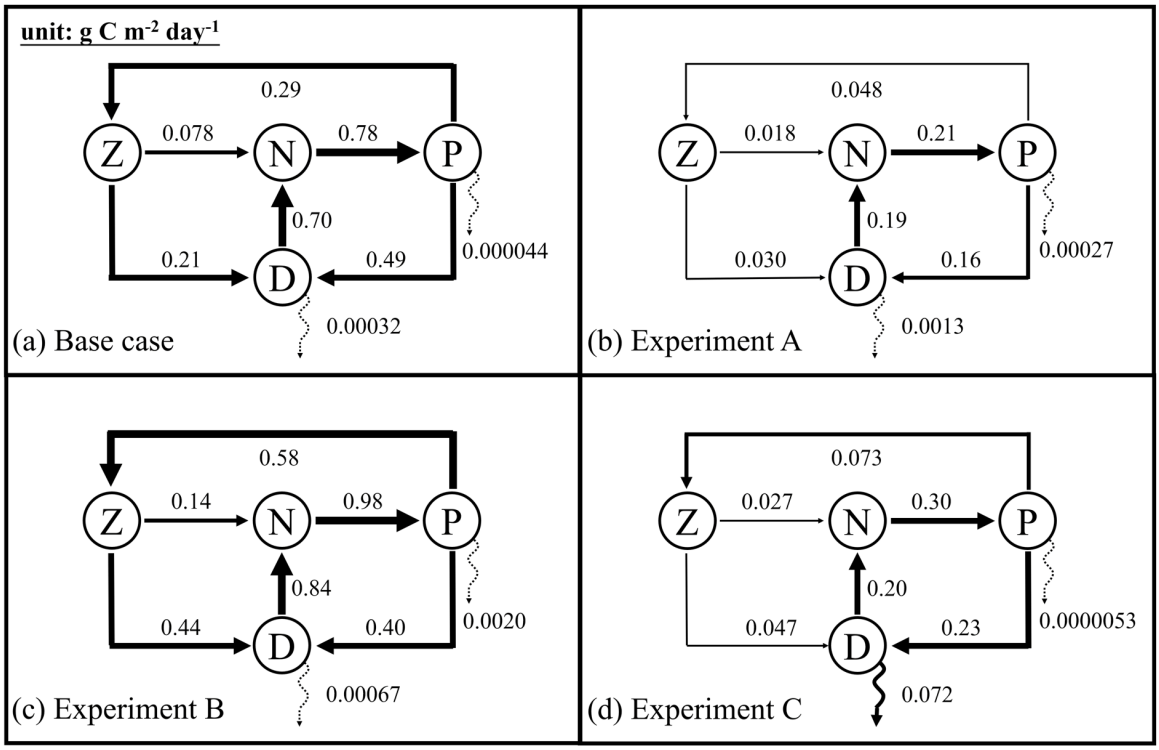

Figure 6. Annually averaged carbon fluxes integrated over the upper 200 m (unit: g C m^{-2} day^{-1}) for the base case (a) and optimized experiments A, B, and C. The N, P, Z, and D stand for the pools of nutrient, phytoplankton, zooplankton, and the sum of small and large detritus, respectively. The thickness of arrows scales with the magnitude of fluxes. Dashed arrows represent fluxes lower than 0.01 g C m^{-2} day^{-1}.

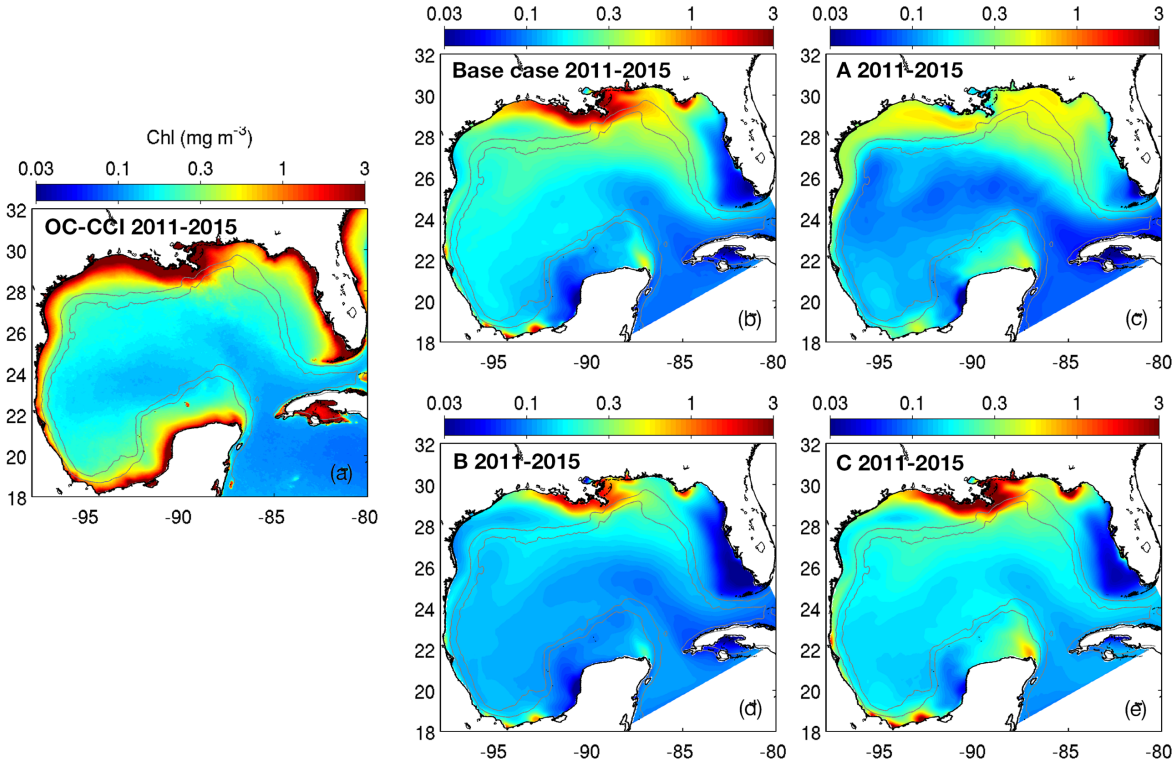

Figure 7. Spatial distributions of the annual mean chlorophyll in the surface layer from the satellite (OC-CCI) climatology (2011-2015) and the different model versions. The gray contours mark the bathymetric depths of 200 and 1000 m.

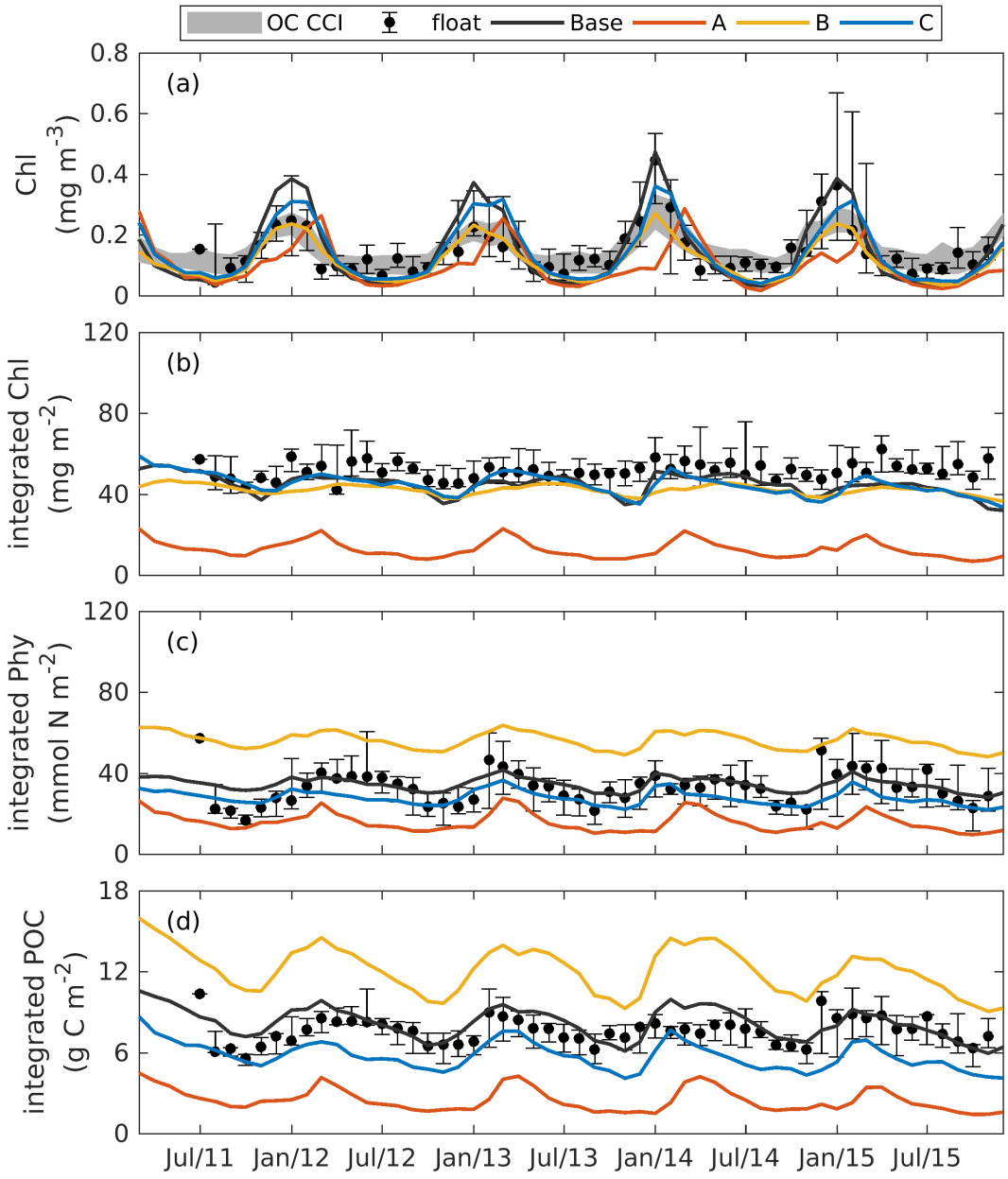

Figure 8. Observed and simulated seasonal cycles of surface chlorophyll (a), vertically integrated chlorophyll (b), vertically integrated phytoplankton (c), and vertically integrated POC (d) from each 3D models. Solid lines represent the median values over the deep ocean of GOM (depth>1000m). Error bars and shades show the 25% and 75% percentiles. Chlorophyll, phytoplankton, and POC are integrated over the top 200m.

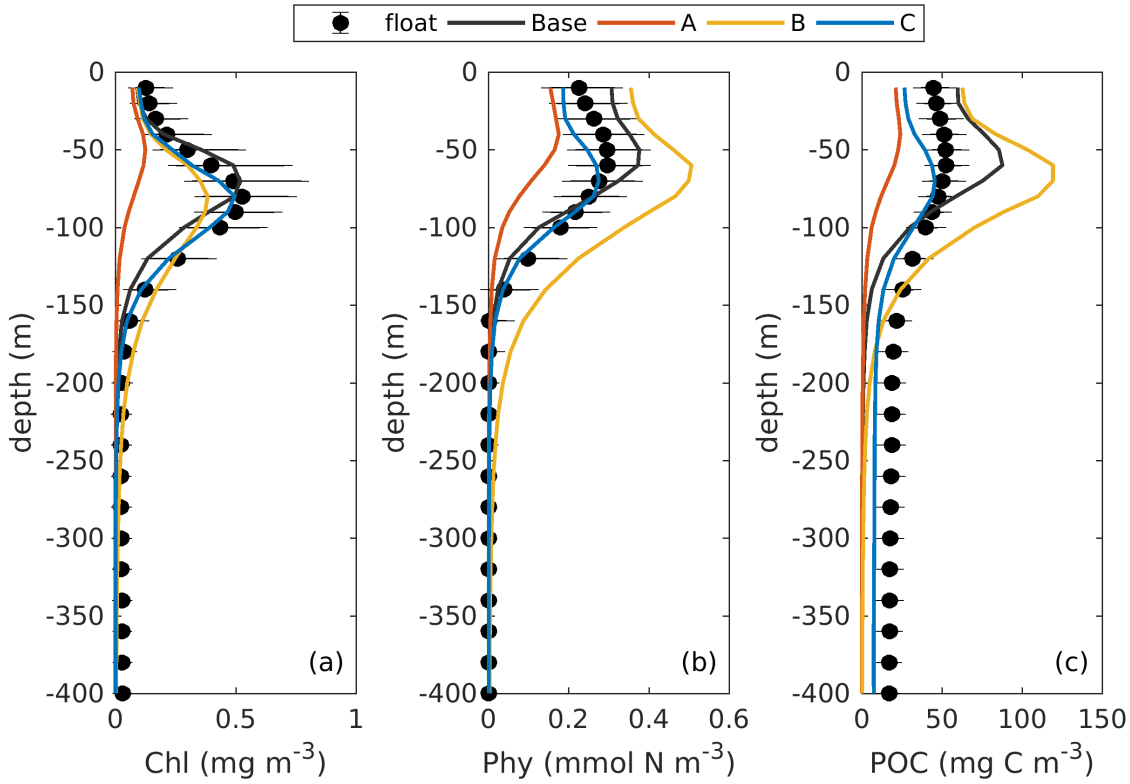

Figure 9. Observed and simulated vertical profiles of chlorophyll, phytoplankton, and POC from each 3D models.

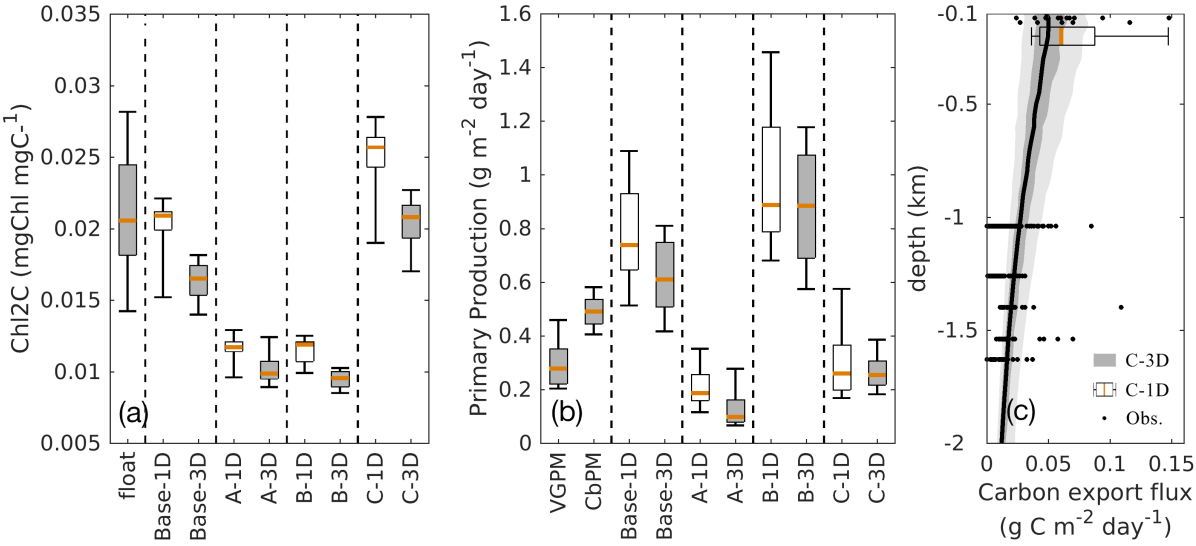

Figure 10. Comparisons of the chlorophyll to carbon ratio (a), primary production (b), and carbon export fluxes (c) between the 1D and 3D models.