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Discussions

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Interactive comment on "Impacts of physical data assimilation on the Global Ocean Carbonate System" *by* L. Visinelli et al.

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Reply to Reviewer 1

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We thank the referee for the careful reading. Following his suggestions, we have modified our previous experimental set-up in the following way:

- We have better described the initialization methods for the model and tested different combination of spin-up procedures. Differently from the previous simulation, the model is now initialized with a 25-years spinup for the physics component only of the OBGCM.

- We used GLODAP initial conditions for the alkalinity.

- We added the $CaCO_3$ cycle and the shell formation/dissolution process in the biogeochemical component.

We have addressed the concerns reported below.

1 General comments

1a) The treatment or better non-treatment of the $CaCO_3$ cycle and thus ALK

is highly cumbersome. Changes in ALK exert a strong control on pCO_2. The authors employ a complex representation to simulate organic matter production and export considering iron, silicate, phosphorus, nitrogen as nutrients and different functional groups from bacteria to zooplankton. They also discuss how variations in S affect ALK. On the other side, and in sharp contrast to the complexity of the ecosystem model, they neglect the first order feature of $CaCO_3$ formation in the euphotic zone and dissolution in the thermocline and deep ocean. In my opinion, it does not make sense to apply a complex ocean circulation model and a complex model for the organic matter cycle in a variational approach, while at the same time neglecting first order drivers of ALK and thus pCO_2 and air-sea flux see e.g. Sarmiento and Gruber ().

We understand the reviewer's concern about the relevance of calcite formation and dissolution processes in the global equilibrium of carbonate species. We originally neglected this process not because of its irrelevance but mostly because the experimental methodology was focused on the role of solubility and transport. We do recognize that temperature also affects the equilibrium constants for calcium carbonate formation and dissolution and that given the complexity of the biological model, a complete treatment of carbonate species is required. We have now redone the entire set of simulations with a version of the BFM model that implements the $CaCO_3$ cycle. The model uses the parameterization proposed by Aumont and Bopp (), which is now described in the revised Sec. 2.2. While the overall inventories of alkalinity and DIC are not particularly affected, we did obtain considerable differences for the surface and sub-surface concentrations (an example for the surface Atlantic is shown in Fig. 1 and Fig. 2). Results have thus changed with respect to the previously submitted simulation, also affecting the resulting distribution of pCO2.

1b) The adjustment of the GLODAP initial ALK fields by 50 micromol in the entire

Pacific is huge. This corresponds to an adjustment in pCO_2 of about 30-50 ppm. How can this be justified?

When revising the entire simulation procedure we found an error in the initial conditions that were supposed to derive from the original GLODAP database. This led to a global offset that required us to implement such an artificial correction (not unusual because also applied for DIC in regional simulations of the Pacific as in Turi et al., 2014). We have now carefully checked the original GLODAP data set and the gridded product to verify that the initial values are in line with the data used for the validation. There is still a mismatch between the initial condition value found in the BATS area and the time series data because BATS data were not included in the original GLODAP product, but we preferred to keep this discrepancy in the new simulations.

1c) It is unclear whether the impact of organic matter formation and dissolution on ALK is taken into account. Please clarify. A proper treatment of the $CaCO_3$ cycle and of ALK is needed before publication.

The $CaCO_3$ cycle and its impact on ALK and organic matter is now taken into account in the model. We have included the following lines in the text, Sec.2.2 "The model includes a simple parameterization of calcite formation and dissolution derived from Ref. (), with the reference phytoplankton content of particulate inorganic carbon (PIC) as estimated by Gehlen (). Calcite is produced by nanoflagellates and released during grazing by micro- and mesozooplankton and the other loss processes involving particulate matter in the cells. The sinking velocity of PIC is set constant to 30 m/d and all processes related to dissolution and formation of calcite lead to the stoichiometric change in the concentration DIC and ALK."

2a) The model is not spun-up towards equilibrium, but run from rest starting in 1988. I am surprised that the model is not properly initialized with a spin-up close to equilibrium as the resolution of the model is with 30 vertical layers and $2 \times (0.5 \div 1)$ degree not as high as to prevent a spin-up. This would allow the authors to evaluate the model's physics and biogeochemistry in a comprehensive way by comparing simulated tracer distributions and water mass formation rates with observations (e.g. GLODAP, World Ocean Atlas, Talley et al. etc), before applying the model in the data assimilation. It would be nice to see a discussion how well the model is performing in terms of simulating nutrient distributions and thermocline ventilation, e.g. as indicated by the distribution of CFCs, radiocarbon or anthropogenic carbon. How does model drift affect results in the control?

We have now better explained the spin-up strategy used for the simulation. We also explored different combinations of spin-up for the physics and carbonate species distribution. The aim of this work was to assess the impact of physical data assimilation on carbonate system dynamics. Data assimilation may indeed be seen as a method to avoid long spin-up phases because observations are dynamically inserted in the model according to the model major modes of variability. Therefore starting from rest is not such an unusual choice for this kind of studies. A spin-up of the physics is however required to improve the results because it allows the system to adjust to forcing functions. However, a combined initialization of physics and biogeochemistry may lead to spurious trends in the carbonate species and CO2 fluxes because of the adjustment of physics. This happens for instance in the case of an excessive evaporation as found in our simulations, an issue that is resolved with the aid of data assimilation as shown in the manuscript (Sec. 3.1). This evaporation leads to an increase of salinity that affects density and the water column is indeed adjusted in the longer term. Such a process does not occur for variables like alkalinity because the initial trend in concentration increase cannot be recovered. For this, see Fig. 3

where we plot the average value of the global surface alkalinity in the spinup, starting from the GLODAP climatological condition. The initial conditions for the carbonate system in the model need to be as close to data as possible. For this reason, as now explained in the revised manuscript in Sec. 2.1 and 2.2, we performed 25 years of spinup of ocean physics, while we initialized the BFM model at rest, starting from the GLODAP for DIC and ALK and the World Ocean Atlas climatologies for nutrients.

2b) I assume that the assimilation of T and S implies adding or removing heat and salt. How do the sources and sinks of heat and salt compare to data-based reconstructions of air-sea heat and freshwater fluxes?

As pointed out, the assimilation of temperature and salinity is a non-conservative procedure. In Figs. 4 and 5, we considered the long-term averages over the first 50m depth of the increments in the heat content and salinity, respectively, due to the 3DVAR data assimilation. These maps provide a qualitative way for interpreting the effects of the assimilation at the surface. Focusing on the tropical regions, we see from these figures that the assimilation scheme adds salt and removes heat. This is consistent with the well-known biases of ERA-Interim due to the over-estimation of short-wave and longwave radiation and of precipitation fluxes (see for example Refs. (; ;)). However, we believe that a discussion of the effects of physical data assimilation on air-sea fluxes is beyond the scope of the manuscript, and would require a deeper analysis.

3a) Why do the authors think that data assimilation is preferred or equally valid to other approaches applied to reconstruct pCO_2 and air-sea fluxes such as atmospheric inversions, neural networks or similar interpolation approaches? A discussion of this point may be useful also in the context of the recent special volume in BG on air-sea fluxes (e.g.; (Schuster et al., 2013;Sarma et al., 2013;Ishii et al., 2014;Lenton et al., 2013;Rodenbeck et al., 2013).

In the Introduction to the article, we added the following comment where we explain why we used data assimilation applied on an ocean and biogeochemical circulation model: "In reconstructing the ocean biogeochemistry, we favored the use of data assimilation applied on a global ocean and biogeochemical model over other methods like atmospheric and ocean inversion because the underlying model uses diagnostic and prognostic equations instead of statistical methods for the physics and biogeochemical fields (; ; ;). Furthermore, since no definitive conclusion has been reached regarding a clearly superior methodology, we believe it is relevant to investigate also alternatives to the approaches mentioned by the reviewer, especially to quantify the uncertainty inherent to the pCO2 reconstruction. This is exactly one of the objectives of the GEOCARBON project which partially funds this work."

3b) Would it be useful to include also the most recent SOCAT version 2 pCO_2 data (Bakker et al., 2013)

We have already used the SOCAT2 data in the previous version of the paper, referring the work by Sabine *et al.* () and using the monthly climatological map. In the latest version of the work, we use the monthly data over the period 1993-2010 (instead of the monthly climatology) to compute the absolute average and the RMSE with respect to the model, and we added the reference to Bakker *et al.* ().

3c) How does this work compare to previous ocean-carbon and air-sea flux data assimilation studies? (e.g.,(Mikaloff Fletcher et al., 2006;Mikaloff Fletcher et al., 2007) (Gerber and Joos, 2010, 2013;Gerber et al., 2009) (Schmittner et al., 2009) (Rodenbeck et al., 2013) or (Schlitzer, 1988, 2004)

All of these work deal with either the surface carbon flux, the detritus flux, or the ocean heat content, which are quantities not discussed in our work. We have added a reference to these work in the Introduction, mentioning the methodologies implemented in their work, without including additional details on the comparison of the carbon flux.

4) Text structure: Metrics should be defined in a subsection of the method section to avoid unnecessary repetitions.

We have moved the metric description into a specific Subsection 2.6.

2 Specific comments

1. **abstract, line 1: The first word in the abstract is "prognostic simulations". I find this a bit misleading as this manuscript deals not at all with prognostic simulations.**
   We removed the term "prognostic".

2. **Methods, section 2.2: a) How are Fe, Si, P, N .. initialized? b) what is the atmospheric pCO_2 boundary?**
   In Subsection 2.2, we added the description of the initialization of nutrients as "Nutrients (phosphates, nitrates, and silica) are initialized with the World Ocean Atlas climatologies" . We had already described pCO_2 boundary in the same section.

3. **p5406, line 15: How do you define the error covariance matrix? Could you describe this a bit in more detail.**

In Subsection 2.3, we added the description of the covariance matrices R and B as "Errors associated with the data set are split into two covariance matrices, the first being a diagonal matrix containing the instrumental and representativity errors associated with the observations, and the second one containing the temperature and salinity background-error covariances, estimated from a set of anomalies with respect to a monthly climatology of a previous non-assimilative run".

4. p5406 Line 23: Is there also a vertical correlation length scale involved? Could you please also specify over which horizontal and vertical domain you assimilate T and S?

In Subsection 2.3, we specified that vertical correlations are implied by the EOFs, while data assimilation is performed considering the whole oceanic region. We added the following text: "The bivariate EOFs have been estimated by the dataset of monthly anomalies with respect to the monthly climatology from an assimilation-free simulation. For the assimilation, we use ten EOF modes for each vertical profile, whose explained variance averaged over the global oceanic region is 98.9%. In order to model horizontal correlations, a 4-iteration first-order recursive filter is used, with a uniform horizontal correlation length-scale equal to 300 Km, while vertical correlation is provided by the EOFs. The OceanVar system also takes advantage of an extended domain with duplicated observations on the symmetric extension zones, which serves the purpose of obtaining cyclic conditions during the application of the recursive filter."

5. 5407, line3/4 Are there physical reason to reject observations? How does this procedure affect the RMSE or similar metrics? Could it be that the practice of throwing away observations yields 'artificially' low RMSE?

We added the description of the rejection method, at the end of Subsection 2.3. "Observational errors are derived from the profiles of instrumental errors in Ref. (), which are subsequently inflated to account for large representativeness errors in correspondence of areas of strong variability. The OceanVar system performs several data quality checks, among which a check against the climatology and a check against background fields that rejects observations with a too large departure from the model fields. In more details, observations are rejected if the square of the misfits between the data and the model outcome is greater than the sum of the quadratic errors of the observation and of the background, times a user-defined constant of the order of ten."

6. 5407, l7: is there no convection?

"Advection" and "convection" refer to the same term in the equation of motion, that is the 3-dimensional divergence term in the total time derivative.

7. 5407 line 10-15: you may see Gerber and Joos, OM, who also assimilated T, S fields

We have added the work by Gerber and Joos (2010) in the introduction, when discussing the models that assess the global carbon flux with the use of data assimilation.

8. 5407, l23, eq. 2: I miss here nitrate alkalinity which should not be neglected. Could you please indicate whether you neglected nitrate alkalinity in the definition of ALK?

We never neglected nitrate alkalinity, which was already included in the BFM code used for the first version of the paper. Now, in the new version of the paper,

we mention that nitrate alkalinity is included under "minor anions" in the equation defining ALK.

9. **15408 line 20: It would be illustrative to provide also the relative change in $p\mathrm{CO_2}$ per change in ALK and DIC**

We have added the formulas for the sensitiveness of the $p\mathrm{CO_2}$ with respect to changes in DIC and ALK concentrations. We added the following text: "The sensitivity of $p\mathrm{CO_2}$ to direct variations in the concentration of DIC and ALK are expressed by

$$\frac{\partial \ln p\mathrm{CO_2}}{\partial \ln \mathrm{DIC}} = \gamma_{\mathrm{DIC}}, \quad \text{and} \quad \frac{\partial \ln p\mathrm{CO_2}}{\partial \ln \mathrm{ALK}} = \gamma_{\mathrm{ALK}}, \tag{1}$$

where γ_{DIC} is known as the Revelle factor. When the contribution of water dissociation to alkalinity can be neglected, an estimation to Eq. (1) is ()

$$\begin{aligned}
\frac{\partial \ln p\mathrm{CO_2}}{\partial \ln \mathrm{DIC}} &\approx \frac{\mathrm{DIC}\,(3\,\mathrm{ALK} - 2\,\mathrm{DIC})}{(2\,\mathrm{DIC} - \mathrm{ALK})\,(\mathrm{ALK} - \mathrm{DIC})}, \\
\frac{\partial \ln p\mathrm{CO_2}}{\partial \ln \mathrm{ALK}} &\approx \frac{\mathrm{ALK}^2}{(2\,\mathrm{DIC} - \mathrm{ALK})\,(\mathrm{ALK} - \mathrm{DIC})}."
\end{aligned} \tag{2}$$

10. **5413, line 15: are there problems with model drift at depth?**

In principle, the assimilation works over the whole profile, but since data become less numerous with increasing depth, at bottom depth we cannot provide the same statistics as for the first 400meters.

11. **section 5: I would prefer here a discussion of results instead a description of metrics. The latter should go to the method section.**

We moved the description of the metrics in the appropriate Subsection 2.6.

12. **5416, eq. 9: Could you define G.**

Before the equation, we have specified that "G_i is the $1^o \times 1^o$ regular SOCAT grid area element associated to the grid point i".

13. **p5417 line 10 to 21. suggest to delete text as it provides hardly any information**

We would prefer to keep this portion of the text, as it provides information on how we performed the computation of the anomalies.

14. **5418 line 5-7: unjustified claim, please delete. It seems not a sufficient require- ments that model performance is just slightly better than when completely neglecting a first order process.**

We removed this portion of the text.

15. **5418, line 19: Mentioning that you neglected the first order process of $\mathrm{CaCO_3}$ formation comes way to late here.**

We have removed this comment since we now include $\mathrm{CaCO_3}$ formation in the code.

16. **5418, line 25: The ad-hoc correction for alkalinity is not justifiable.**

We removed the ALK correction in the Pacific, using now the GLODAP climatology.

17. **5427: table 1 is not needed**

    We would prefer to keep Table 1 in the text as a quick reference for the experiments.

18. **Figure 2: It seems you are comparing to station data. The labels 'GLOBAL', 'Atlantic' etc are then very misleading. Please use other labels (e.g. TOGA-TAO) etc. What means 'GLOBAL'**

    We relabeled the figures with the appropriate floats names. We added the following description: "The label "GLOBAL" refers to the RMSE computed by using the complete set of *in-situ* data used in the reanalysis from different types of instruments, accounting for all data that have not been rejected by the 3DVAR scheme and over the whole vertical profile. "

19. **figure 2: What about pCO_2? Please show also RMSE for pCO_2, e.g. as compared to SOCAT version 2 data.**

    We already included the pCO_2 RMSE in table 5. We now perform the RMSE using monthly data, instead of climatological months.

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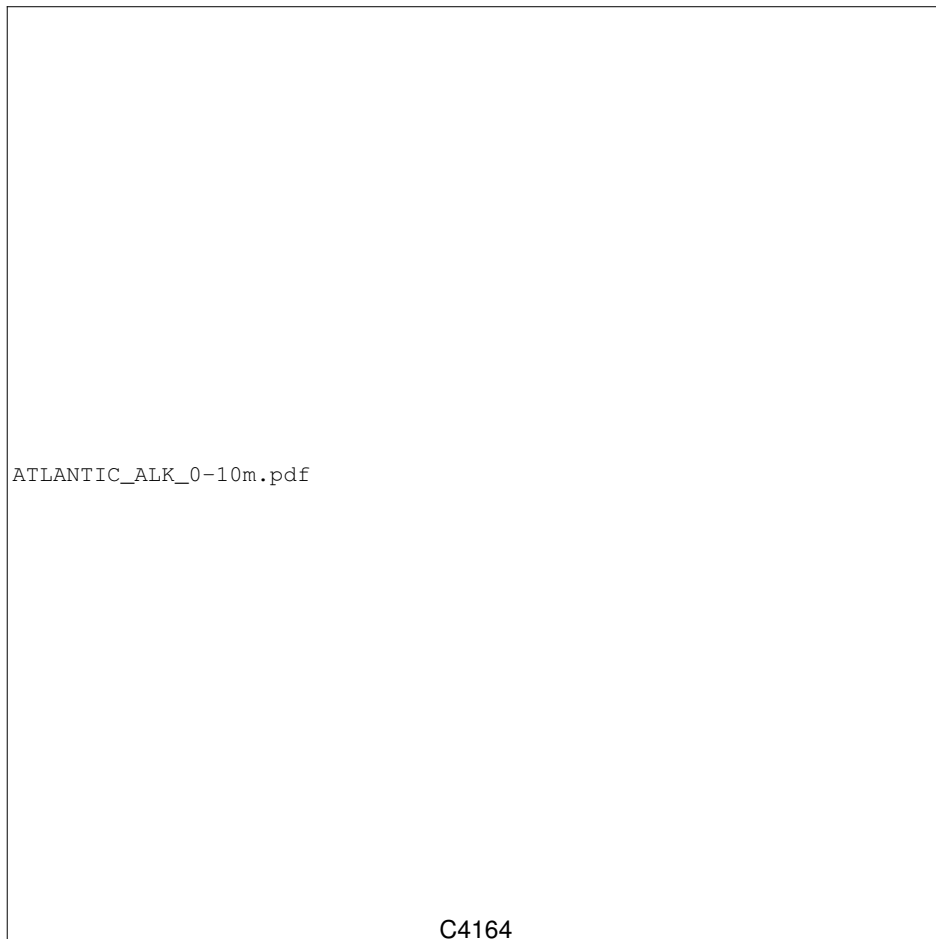
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C4163

ATLANTIC_ALK_0-10m.pdf

C4164

Fig. 1. Sea surface alkalinity in the Atlantic ocean from the reanalysis run, when CaCO₃ cycle

ATLANTIC_DIC_0-10m.pdf

C4165

Fig. 2. Sea surface DIC in the Atlantic ocean from the reanalysis run, when the CaCO₃ cycle

spinup_ALK.pdf

C4166

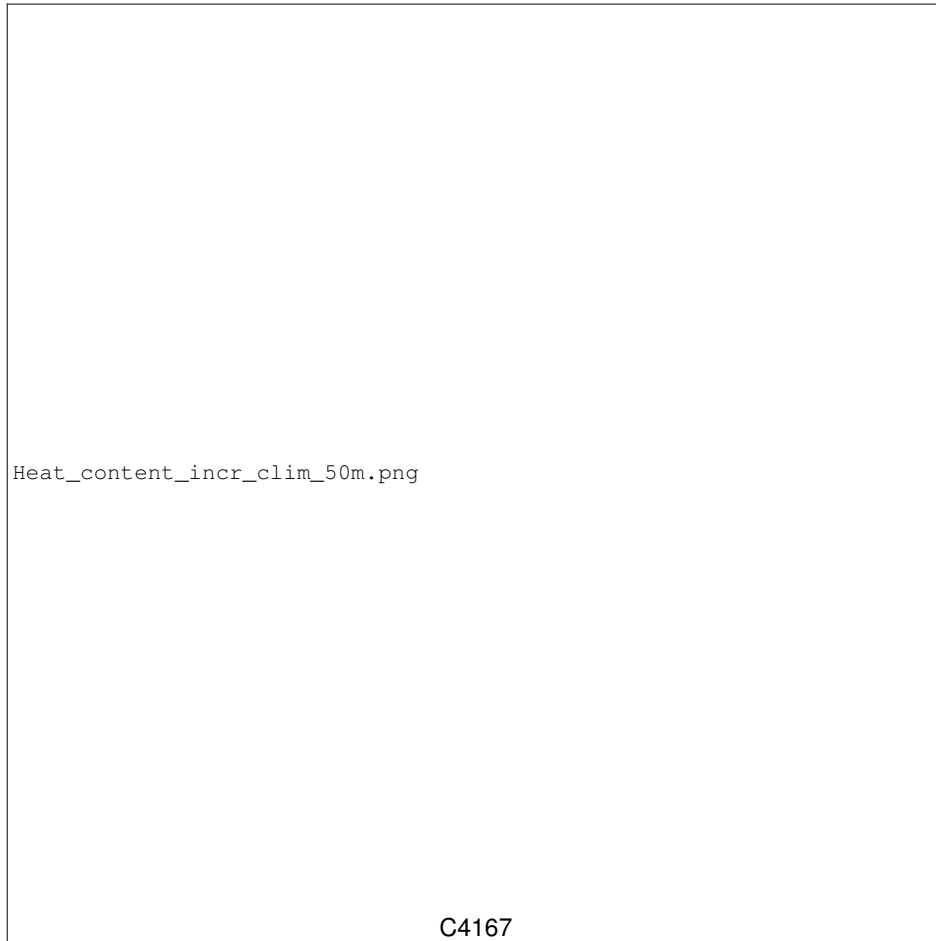**Fig. 3.** Surface alkalinity during spinup, averaged over the global ocean area

Heat_content_incr_clim_50m.png

C4167

Fig. 4. Climatological map showing the increment in the heat content implied by data assimila

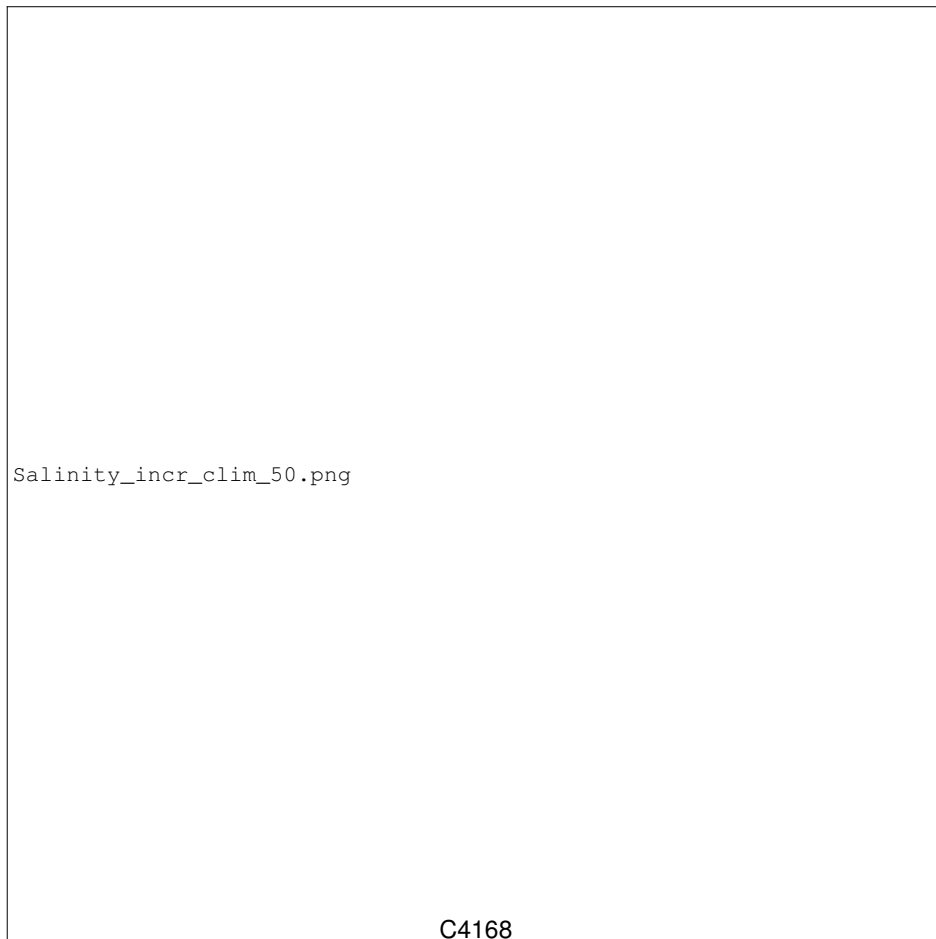Salinity_incr_clim_50.png

C4168

Fig. 5. Climatological map showing the increment in the salinity implied by data assimilation