Reviewer 1

This work addresses the general issue of taking best advantage from dense and highresolution satellite observations, in particular satellite sea surface salinity (SSS) data, to improve our prediction and knowledge of ocean dynamics. One main difficulty relates to the large discrepancies between observation and forecast ensembles that can appear in frontal regions due to mismatches of the sky type (clear versus cloudy). These large discrepancies may induce unphysical analysis corrections in frontal regions. To overcome this issue, the objective of this study is to adapt the AOEI method (adaptive observation error inflation based on Desroziers' innovation diagnostics) to an EnKF-based ocean data assimilation (3D-LETKF formulation with 100 members). The AOEI provides thereby a way to inflate observations errors with a spatial dependency. In this paper, the Authors study the AOEI impact on salinity structure, geostrophic balance and accuracy in the northwestern Pacific region when all-sky infrared brightness temperatures are assimilated at one-day time intervals. They illustrate the degradation of the salinity structure resulting from EnKF analysis without AOEI and impacting vertical diffusion. They also demonstrate that including AOEI within the EnKF can successfully limit the erroneous analysis increments and thereby preserve the salinity structure.

I find that the paper is generally well written and clear. The issue raised in this work is of great interest for the geoscience community because it is essential to be able to take advantage of current and future satellite observations to improve model predictions. The case study and results are relevant to answer this question. I also find that the introduction shall put more emphasis on the objectives and on the issues associated with data assimilation when dealing with structures/patterns and therefore position errors. This is a general problem of standard data assimilation algorithms, which have been designed to handle amplitude errors and not position errors. The AOEI method provides a way to limit the issues of position errors in areas where observation errors may also be large. However, it would be of interest to readers to replace this issue in the more general context of position error treatment in data assimilation systems. Adding some comments in the introduction and conclusion on this aspect would be worthwhile.

We thank the reviewer for insightful comments, especially on the position error. We have added the description of the differences in the position of the boundary between forecasts and observations to the third paragraph in Sect. 1.

By the way, I find that the paragraph "As shown in section 3, an EnKF-based ocean data assimilation system... are large due to fronts and eddies." (1. 69-72) is not at the right place

in the introduction. It is surprising to announce in quite significant details the results found in the paper directly in the introduction. I suggest the Authors to modify/reformulate this part to further discuss the idea of position errors. Also, in lines 325-329, there is a discussion on the limits of the SST, SSS and SSH assimilation due to the prescribed vertical localization scale. It is not clear in the text if this limit is satisfying or if there is some work to be done to overcome this limitation. How was this localization scale defined? How does it impact the vertical diffusion processes discussed in the paper? Comment on this aspect would be valuable.

In the third paragraph in Sect. 1, we have removed the description of the salinity degradation seen in the experiment, and added the general insight on the similarities of ocean fronts to the atmospheric boundaries between clear- and cloudy-sky, following the reviewer's comments.

We have conducted preliminary experiments with and without the vertical localization scale. We have found that the low-salinity structure is more likely broken in the experiment without vertical localization than that with vertical localization, probably because assimilating surface observations results in the larger analysis increments throughout the depth and causes the degradation mechanism. Therefore, we have set the vertical localization scale of 100 m following Miyazawa et al. (2012) and Penny et al. (2013). As described in the last paragraph in Sect. 4 in the original and revised manuscripts, the horizontal and vertical localization scales are not optimally tuned in this study, and this is an issue in future studies.

(*) Some additional minor comments

We thank the reviewer for checking carefully throughout the manuscript. We have modified corresponding parts following your comments.

I encourage the Authors to

- Throughout the manuscript, change "1 day" to "one day"

We have replaced "1 day" with "one day" in the Abstract, the third paragraph in Sect. 1, and the second paragraph in subsection 2.2.

- Throughout the manuscript, write "Section" with a capital letter at the beginning of sentences, and use the abbreviation "Sect." within sentences.

We have replaced "section" with "Sect." in the last paragraph in Sect. 1 and in the last sentence in subsection 2.1.

- 1. 15, correct typographical error "by combining forecasts and observations"

We have replaced "bv" with "by" in the first sentence in the first paragraph in Sect. 1.

- 1. 40, add references related to variational approaches for ocean data assimilation

At the end of the first paragraph in Sect. 1, we have added the citation of Miyazawa et al. (2017) and Zuo et al. (2019) in which 3D-VAR is adopted in ocean data assimilation systems.

- l. 42, correct grammar error "provide a large number"

We have replaced "provides" with "provide" in the second paragraph in Sect. 1.

- l. 147, remove the reference Ohishi et al. (in preparation): it is not conventional to cite a paper that is in preparation, it should be at least accessible in some ways.

In the first sentence in subsection 2.3, we have incorrectly cited Ohishi et al. (in preparation), and replaced "Ohishi et al. (in preparation)" with "Ohishi et al. (in review)". In the last sentence of Sect. 4, we have removed "Ohishi et al. (in prep.)".

- 1. 169, remove the word "taking"

We have removed "taking" between "By" and " $\partial/\partial x$ " in the second sentence in subsection 2.3.1.

- 1. 171, precise what is meant by "the accuracy" (the accuracy of what?)

We have added "of temperature, salinity, horizontal velocities, and SSH" after "the accuracy" in the first sentence of subsection 2.3.2.

- 1. 350, define the acronym SSHA the first time it appears in the text

We have added "(SSHAs)" after "sea surface height (SSH) anomalies" in the last sentence of the second paragraph in Sect. 1.

- Bibliography, modify the year for reference by Desroziers et al. (2005)

We have incorrectly cited Desroziers et al. (2006), and therefore replaced "Desroziers et al. (2006)" with "Desroziers et al. (2005)" in the third paragraph in Sect. 1, in the first sentence in subsection 2.1, and in References.

Reviewer 2

The authors propose to use a novel extension for the use of ensemble Kalman filters (EnKF) in a pre-operational ocean reanalysis product. The adaptive observation error inflation, previously introduced for satellite data assimilation, reduces assimilation increments by automatically inflating observational errors. The results show this automatic inflation as improvement compared to static observational errors. These results hold especially at Ocean frontal zones, where a large vertical diffusion can be observed with a static covariance. In general, this idea is relevant to improve data assimilation/reanalyses with ensemble Kalman filters, and the manuscript is well-written. Nevertheless, the manuscript needs a revision in its current form, at least with more and longer discussions, especially in relation to the number of figures. Also, the manuscript is not totally self-contained.

We thank the reviewer for constructive comments. We have replied to your comments in the following.

1) Whereas the ensemble Kalman filter, its assumptions, and its equations, are wellknown, adaptive observation error inflation is quite unknown in the literature. Although the authors state and shortly explain the relevant equations, the explanations for this technique are too short. Its assumption and when we would expect that it works well remains totally unknown. Based on Desroziers et al., 2005 (often cited as 2005 and not 2006, which might confuse an informed reader), the relationship within the innovation statistics assumes Gaussian background and observational errors as in the ensemble Kalman filter, but what happens if these assumptions are violated?

We have incorrectly represented Desroziers et al. (2005) as Desroziers et al. (2006), and therefore replaced "Desroziers et al. (2006)" with "Desroziers et al. (2005)". As clear from Eq. (2), no correlation between forecast and observation errors is assumed in the formulation of the innovation statistics, and no assumption that the forecast and observation errors follow the Gaussian distribution is applied.

As indicated by the reviewer, the forecast and observation errors are assumed to follow the Gaussian distribution in the EnKF, but the effects of the forecast and observation errors not following the Gaussian distribution on the EnKF are beyond the scope of this study.

In addition, a crucial assumption is the correct representation of the background error

covariance with the ensemble; only then, Equation (1) represents a correct observational error covariance. The heavy use of relaxation to prior perturbations (RTPP) shows difficulties with the ensemble spread and I wonder if the ensemble spread is correctly tuned, especially in the Ocean frontal zones. The use of the maximum between estimated covariance and prescribed covariance lessens possible problems with these assumptions, but nevertheless, they should be named and discussed in the manuscript.

The equation from Desroziers et al. is only valid in expectation of the errors. For me, it remains unclear if and how this expectation is built in the data assimilation system. If no expectation is used, then its consequences and its connection to quality control and robust assimilation should be discussed, e.g., what happens in different innovation magnitude regimes (smaller or larger than the expected innovation magnitude)? In total, the method part of the adaptive observational error inflation needs to be revised.

As described in the first paragraph in subsection 2.2 in the original and revised manuscripts, we apply the perturbed atmospheric and lateral boundary conditions to the EnKF-based ocean data assimilation system to avoid filter divergence, following Ohishi et al. (in review) (See subsection 2.2 in Ohishi et al. in review). Ohishi et al. (in review) demonstrated that the combination of the IAU and RTPP with 80–90 % relaxation results in the best dynamical balance and accuracy, and therefore the RTPP parameter has been tuned in the experiments with fixed observation errors. However, because of the limitation of the computational resources, the tuning of the perturbed boundary conditions and RTPP parameter in the experiments with the AOEI is beyond the purpose of this study, as described in the last paragraph in Sect. 4.

We thank the reviewer for indicating statistical expectation and accuracy for the forecast ensemble spreads. We have added the statistical expectation to the LHS in Eq. (1). As indicated by the reviewer, the AOEI assumes that the forecast ensemble spreads are correct and the residual in Eq. (1) is caused by underestimation of the observation errors, and that $(d_b^o)^2$ is assumed to be equivalent to $\langle (d_b^o)^2 \rangle$ in Eq. (2). To mitigate underestimation of the estimated observation errors, the larger observation errors between the estimated and prescribed errors are chosen as shown in Eq. (3). We have added the assumptions used in the AOEI to the end of subsection 2.1.

2) The results show an improvement with adaptive observation error inflation compared to a static observational error assumption. The static observational errors results into too large assimilation increments and, thus, to a strong vertical diffusion at the Ocean frontal zones. As the static observational error covariances are important for increments, its magnitudes are very important. Although the numbers are stated, their sources remains unknown. Because of the missing sources, the reader is unable to know if the prescribed uncertainties come only from the uncertainties of the observational products or if they also include other uncertainty sources like the observation operator or the representation error. The results indicate a larger representation error at the Ocean frontal zones than included in the observational error. A usual approach would be thus to generally inflate the observational errors or to withheld observations in these zones. Consequently, I would wish for a comparison experiment with an inflated observational error (e.g., 2 times the stated observational error) to see if a proper tuning of the errors would lead to better scores and how this might help in the case of the frontal zones. The authors have stated that they have only a limited computational budget, and a proper tuning of the observational errors and/or a comparison experiment might be too expensive. It might be therefore also enough to explain more in detail the advantages and disadvantages of adaptive observation error inflation compared to a tuned observational error, which can be again related to the discussion in point 1 of this review. Although the results seem to be good, the reader could be generally tempted to believe that the results are only caused by a nontuned assimilation system.

We have compared the accuracy of the experiment with larger temperature observation error of 1.5 °C (denoted as 1.5Terr run hereafter) conducted in Ohishi et al. (in review), the CTL run with 1.0°C observation errors, and the AOEI run. For example, the RMSDs of the CTL, AOEI, and 1.5Terr runs relative to the drifter buoys are 0.260, 0.257, and 0.258 m s⁻¹ for surface zonal velocity, and 0.250, 0.248, and 0.249 m s⁻¹, respectively, and therefore the accuracy of the AOEI run is the best. We have added the description at the end of subsection 3.4 in the revised manuscript.

The following is my opinion for EnKF-based ocean data assimilation systems. Even if the perturbed boundary conditions are applied, the ensemble spread is small and assimilation impacts tend to be small in the subtropical region. To increase the assimilation impacts in the subtropical region, one might think that setting the smaller observation errors are better. However, small observation errors result in the degradation mechanisms in the frontal regions as seen in this study. The AOEI plays a role in suppressing the degradation mechanism if the small observation errors are set.

3) In general, the results part would profit a lot on concentrating on the most important parts of the study. Although well-written, the amount of figures compared to the discussion makes it difficult to follow the red line in the results part. Sometimes, similar

information is shown twice (e.g., Figure 6-8) and could be condensed into a single figure. Caused by the difficulties to follow the red line and a rather loose summary section, the main message of the manuscript remains also slightly unclear for me. On the one hand, this study tries to show how the static observational error induces problems with the vertical diffusion. On the other hand, it promotes of how adaptive observational error inflation can help. As discussed in section 2 of this review, the sensitivity experiments might be not enough to promote adaptive error inflation and to cancel out difficulties with the static observational error.

I like how the authors explain their evaluation in detail within the results part, but in its current form, it distracts from the main results and is too long. I would recommend to give here only concise explanations of the evaluation and to move specific equations and details into the appendix.

All of the descriptions, figures, and equations included in the manuscript are essential to reveal how the AOEI improves low-salinity structure. The degradation mechanism in the CTL run is quantitatively investigated in subsection 3.1, how frequency and where the AOEI is applied is shown in subsection 3.2, and the improvement mechanism by the AOEI is quantitatively investigated in subsection 3.3. The detail of the degradation mechanism in the CTL run and improvement mechanism by the AOEI would be useful for readers when they establish an EnKF-based ocean data assimilation system and face the similar problems. To clarify the story in Sect. 3, we have added the descriptions between Sect. 3 and subsection 3.1, and we have maintained the contents in the manuscript.

Smaller comments:

As an advice, the chosen colormaps might be generally misleading and inaccessible for colour-blind persons. In addition, the same colours are used for different meanings in subfigures (e.g. Figure 5), which can be also very misleading for the reader.

As indicated by the reviewer, we have modified the color of the solid lines in Fig. 5a (11a) to distinguish between the colors of Fig. 5a (11a) and Fig. 5b, c (11b, c).

I would be interested into a comparison experiment without any data assimilation, except for example SST and SSH nudging as done for the spin-up phase. Currently, it remains unclear for me if the noisier pattern in the SST fields compared to observations are caused by the data assimilation or if this is a "natural feature" of the model. This could be even shortly stated in the results part and then simply shown in a supplementary material or if this was discussed in the other manuscript, then the authors could simply point this fact to the other submission. In this sense also the naming of the experiments is a little bit confusing as the "control" run is usually an open-loop run without data assimilation whereas here it describes the baseline EnKF experiment, I would rename it into EnKF or STATIC.

We have confirmed that the noisy SST and SSS signals and degradation of the low-salinity structure do not appear during the spin-up period. We have added the description at the end of the first paragraph in subsection 3.1.

The CTL run is well used to compare between experiments with and without schemes even in data assimilation systems (e.g. Kotsuki et al. 2017; Zuo et al. 2019), and therefore we have maintained the name of the CTL run.

The authors frame the introduction as there are only two previous works on the EnKF for the Ocean. It might be correct that there are only two reanalysis products based on the EnKF but there is surely more work on the EnKF for the Ocean.

As summarized in Ohishi et al. (in review), the EnKF is implemented with ocean data assimilation systems, but only two EnKF-based ocean reanalysis datasets exist to the best of our knowledge. To clarify that there are many ocean data assimilation systems with EnKF, we have added "(See table 1 of Ohishi et al. in review)" after "The EnKF has the advantage of being easy to implement for various models" in the first paragraph in Sect. 1.

In line 133, the authors state that they use covariance localisation. This term might be misleading, as they seem to use observational (covariance) localisation. I would rename it into R-matrix localisation as normally used in ensemble Kalman filter literature. In line 136, the use of incremental analysis updates (IAU) is indicated. The sentence links the use of IAU to ensemble inflation, which is not its normal use in ensemble Kalman filters. I would thus split the sentence with IAU and RTPP into two sentences. In addition, it is unclear how IAU is applied, if for example the increments are applied before and after the original time point or only after etc.

To clarify that covariance localization is applied in the observation space, we have added "in the observation space" after "Covariance localization" in the second paragraph in subsection 2.2.

As described in the original and revised manuscripts, Ohishi et al. demonstrated that the combination of the IAU and RTPP results in the best dynamical balance and accuracy, and therefore we have maintained that "the combination of the IAU (Bloom et al., 1996) and RTPP (Kotsuki et al., 2017; Zhang et al., 2004)". Here, Ohishi et al. (in review) have described the detail of how the IAU is applied, and therefore we have added "; Ohishi et al. in review" after "Bloom et al., 1996" in the second paragraph in subsection 2.2.

In line 143, "the" SSS nudging is named, what is "the" SSS nudging? Is it the same nudging as used for the spin-up phase? If yes, please state this explicitly.

We have used the same SSS nudging as the spin-up period in the CTL and AOEI runs, and added "as in the spin-up period" at the end of the last paragraph in subsection 2.2.

Other, smaller, issues could be resolved after a revision round.

Reference:

Ohishi S, Hihara T, Aiki H, Ishizaka J, Miyazawa, Y, Kachi M, and Miyoshi T.: An ensemble Kalman filter system with the Stony Brook Parallel Ocean Model v1.0, Geosci. Model Dev. Discuss. [preprint], https://doi.org/10.5194/gmd-2022-40, in review, 2022. Zuo H, Balmaseda MA, Tietsche S, et al (2019) The ECMWF operational ensemble reanalysis–analysis system for ocean and sea ice: a description of the system and assessment. Ocean Sci 15:779–808. <u>https://doi.org/10.5194/os-15-779-2019</u>