

Ocean Sci. Discuss., author comment AC3
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Reply on RC3

David S. Trossman et al.

Author comment on "Tracer and observationally derived constraints on diapycnal diffusivities in an ocean state estimate" by David S. Trossman et al., Ocean Sci. Discuss., <https://doi.org/10.5194/os-2021-87-AC3>, 2022

(Our responses are in boldface below:)

•The paper seeks to evaluate if we can improve oceanic mixing estimates on a global scale by considering assimilation constraints to some novel ocean parameters - diapycnal diffusivities (k_p) and dissolved oxygen. To do that, the authors used an assimilation framework (mitGCM/ECCO), a biogeochemical model (BLING) and a reduced order cost function to estimate sensitivities of numerical parameters in an idealised assimilation scenario. The author concluded that a) a global analysis using only classical ocean observations stays at min. 1 order away from in-situ, b) that the possible "innovations" by assimilating k_p can reduce/increase k_p in important regions and that most regions are in agreement with "innovations" driven by oxygen alone and c) that oxygen seems to provide extra information to constraint k_p . The paper is well structured, concise, the English are clear, and the description of results are cohesive with figures/the general presentation/discussion. However, in my opinion, the paper lacks in detail and suffer from some oversimplifications, omissions, and insufficient discussion regarding some choices/results. The paper is 20% results/discussion but still lack important details to interpret the results. I felt the text missed on important aspects, which are skipped, not even mentioned at all, or mentioned too late - this mostly occurs at Introduction/Methods, but also in results. My major concern is that a lot of details are missing discussion: Aspects of K_p parametrisation in the MIT ocean are lacking, a priori decisions in terms of the inversion. The authors appear to know well the details of the observations estimates but not much detail is provided in terms of the numerical model. My point here is that some information or estimates are sprinkled throughout the text or the next session, generating a back-forth reading and raising too many questions along the way - causing the user to try to build bread from crumbs. I think the authors need to reorganize the paper again - the paper reads like an incomplete explorative analysis, without good justifications or reasoning regarding decisions and the way the work was set up - maybe this was chopped off? The abstract need a lift-up - it is not complete and could be more

laser-focused. Results: There are some good insights here and there, but I found the paper lacks important milestones along the sections to put the reader in the right mindset. Datasets are barely presented, figures are not self-described. What each simulation is using/how it is performed is very rushed and not clear from the start. The aspects of assimilation are not evenly formally described. Although I'm not a specialist in the ECCO model, the description here lacks enough detail. Maybe the author wished to simplify, but I think it end up cutting too much!?. Some de-facto nomenclature in data assimilation is brushed and only add to the confusion to the ones not familiar with ECCO. In short, I think the paper deserves a major review, mostly for clarity of what has been done and to reduce the guesswork, raised questions, and mental gymnastics from the reader. In general, I believe the paper results may be actual good results, there are some good insights, but the lack of attention to detail and description of what was performed put me in the uncomfortable position of having one step back in trusting it. The shallow and rushy discussion at the end with all the caveats clobbered together without any linkage is disheartened. Finally, there is an appendix that contains more description/methods/results which although related to the paper, do not link well to the text/results - there is only a single reference out of context. The author does not explore the aspects of the appendix results and the main research topic - it appears as just a dump of information. I would remove or overhaul the text to point to the results presented in the appendix.

•Thank you for the detailed review. We have worked to clarify the abstract, describe the data sets and ECCO, better streamline the caveats, and link the Appendix with the main text. Specific edits based on your comments are listed below. We hope you find the manuscript to be improved.

Specific comments

•Below you will find some informal notes/suggestions with my personal opinion that I hope will help the author to be more clearer and better understand more points of view of the work. These notes were made mostly in chronological order, so some aspects are discussed in a rolled/back forth fashion. Although some are a matter of opinion, I'm certain that at least some of them can help improve the paper. 3-4: "is not sufficient to constraint K_p ". I would disagree - if the K_p is being analysed/is part of the state vector/changes at analysis time, it is being constrained. This is using a lax formalism of "constraint" - which doesn't bode well with an assimilation subject paper.

•We should point out that there are important differences between the sequential data assimilation systems you are thinking of and the parameter and state estimation framework we're using in the main portion of the text here. We separate out the two different types of observationally constrained modeling systems into the main text and Appendix to be clear about this. The parameter and state estimation framework we use (ECCO) uses observational constraints to estimate parameters and initial conditions. The "analysis time" is the entire length of the model simulation, which should be contrasted with the ten-daily analysis time of the GMAO S2S data assimilation system we use in the Appendix. We are only suggesting that oxygen provides information about $\kappa\rho$ here because we're comparing adjoint sensitivities and not actually "assimilating" the oxygen. While oxygen is included in the cost function in ECCO, this is not the same as estimating the parameters and initial conditions with an optimization run with ECCO, nor is this the same as assimilating oxygen with a sequential data assimilation system to calculate analysis increments. The adjoint sensitivity approach we use in our manuscript can rule out whether a data set, like oxygen concentrations from WOA13, provides information about a particular parameter, like $\kappa\rho$, but our main result is that we cannot rule out this possibility. We cannot make a stronger conclusion, though, because we have not performed the parameter and state estimate optimization with all observational data sets included in the cost function. This is why we have the language we used in the abstract. We have attempted to clarify that these three types of simulations are very distinct and each can provide information, but for different applications.

• 5-10: I would rewrite this.

•Saying “assimilated” in any ECCO-related context should be changed to “included in the cost function” in our manuscript. This is because the parameter and state estimation framework is not a data assimilation framework in the sense most people think about it. The adjoint inverts for parameters and initial conditions using observational constraints instead of adjusting its state using increments (as a sequential data assimilation system would). You could think about ECCO as a long-term 4D-VAR framework but the way we are using ECCO in this study is as a framework that allows us to assess the similarities between sensitivities of the cost function to a model parameter. We have rewritten most of the abstract and hope that this resolves at least some of the confusion. We say, “... we show that the inclusion of misfits to observed physical variables—such as in situ temperature, salinity, and pressure—currently accounted for in ECCO is not sufficient to constrain $\kappa\rho$, as $\kappa\rho$ from ECCO does not agree closely with any observationally-derived product.”

•12: What about $\kappa\rho$ misfits?

•We compare simulations with $\kappa\rho$ misfits to simulations with oxygen misfits in our manuscript, which we now clarify this with our rewrite of the abstract now. We say, “[w]ith the goal of improving the representation of $\kappa\rho$ in ECCO, we investigate whether adjustments in $\kappa\rho$ due to inclusion of misfits to a tracer—dissolved oxygen concentrations from an annual climatology—would be similar to those due to inclusion of misfits to observationally-derived $\kappa\rho$ products.”

•14-15: Why? Describe why - including in the results (see notes below).

•In the abstract we now explain why with our last sentence, "... we show that adjoint sensitivities of dissolved oxygen concentration misfits to the state estimate's control space typically direct k_p to improve relative to the observationally-derived and microstructure-inferred values."

•54-60: Here is a good opportunity to introduce how ecco state estimate works differently from others and if the configuration you use is dynamical consistent instead of what is being said.

•We have added the following sentences, "These control variables can be iteratively improved by running the model in forward and backward- its "adjoint"-modes, which enables the calculation of gradients in the cost function. Each of these runs maintains dynamical and kinematical consistency because, in contrast to sequential data assimilation systems (see the Appendix for an example), the only variables that get adjusted are the control variables, not the dynamically and kinematically active variables."

•69-72: I don't understand this focus here. Data assimilation could account for structural and measurement errors - you just need to adapt the observational error in the equation, inflate/deflate errors according to the product.

•It's true that this is one way to resolve the problem with the combination of both measurement and structural errors. However, the equation you would adapt the observational error into in this case requires vertical resolution finer than the model's grid. We mention in the conclusions a potential way to assess the structural errors: compare CTD-derived k_p using the finescale turbulence parameterization with microstructure-inferred k_p where each of these measurements are co-located. These k_p agree, on average, to within 2%, but there are spatial disagreements, depending upon the vertical bin sizes chosen, and the fidelity of the CTD data is currently unknown. The structural errors associated with the finescale turbulence parameterization's k_p would only be a guess right now.

•73-74: Humm... these lax definitions are unnecessary if you define it more formally above.

•The adjoint is just the model being run backwards. We define what the adjoint is a bit earlier in the text now, but its formal definition is just the model code being run in reverse.

•80:85: I wonder if this distinction is actually necessary here and the paper in general (in

sensitivity terms). For example, you say you use different k_p obs sources in the K_p experiment, but you assign a constant error for both (apparently).

•The distinction is necessary for the reader to be reminded of because the errors assigned to the inferred/derived products of k_p are approximate, whereas the measurement errors for quantities like dissolved oxygen concentrations are more well-known. Further, the derived k_p are based on Argo and CTD measurements that are used in a theory that requires spectral calculations, whereas the inferred k_p are based on microstructure measurements that are used in a simple relationship. We wanted to distinguish between “inferred” and “derived” because the microstructure-inferred k_p is considered the gold standard that (virtually?) every oceanographer trusts. We compared the other observationally-derived k_p with the microstructure-inferred k_p for this reason.

•83: which method?

•We were referring to the finescale turbulence parameterization here. We have clarified this in the text.

•85-115: I understand you want to distinguish the observations and how they are derived, but for the assimilation what is important is the error you assign to the respective obs set. The nomenclature of K_p is a bit jarring too. K_p from a free-run (missing), the K_p from the state estimate at the start (missing), K_p after iteration 59 (I assumed here and thereafter K_p ECCO), K_p micro, K_p w15, K_p K17.

•The κ_p from a free-run (E-CTRL) is the κ_p after iteration 59. ECCO estimates κ_p over the 59 iterations and that κ_p is used for the re-runs. κ_p ,ECCO always refers to κ_p after iteration 59 in the text. κ_p from the first iteration is also discussed in the text, though, so we have let κ_p ,ECCO,0 be this κ_p .

•95/110-115: I miss a figure here showing these observations estimates in a simple way - you got 3 different estimates, 1 gridded, 2 scattered. This would be a figure.

•We now include a figure that shows the gridded initial conditions of O2 for the ECCO simulations, the difference between the initial conditions and the WOA13 product where observations were taken (depth-averaged—as in the previous draft of the manuscript), and a pointwise scatterplot between the initial conditions and the WOA13 product where observations were taken.

- Better yet if shows the actual K_p from ECCO which is absent and we know nothing about the spatial variability. There is not a good picture of obs coverage in the paper.

- **We show the Argo-derived $\kappa\rho$ and how this differs from the ECCO-estimated $\kappa\rho$. The maps that show how these two differ also have the locations where microstructure observations were taken. It is important to show the Argo-derived $\kappa\rho$ because this shows the coverage. We show the profiles of $\kappa\rho$ from ECCO over 16 different example microstructure campaigns and averaged over all microstructure campaigns. We now also show the de Lavergne et al. (2020) $\kappa\rho$ and how this differs from the ECCO-estimated $\kappa\rho$. So we show the observational coverage, but we haven't explicitly shown the $\kappa\rho$ from ECCO in a map (only sampled profiles and maps of differences). We now include a figure of $\kappa\rho$ from ECCO averaged over all depths below the mixed layer (because if the mixed layer is included, then $\kappa\rho$ wouldn't be representative of values anywhere but inside the mixed layer).**

- 123: Describe what the Oxygen from WOA is, units, coverage, mean/standard deviation figure? Limitations? What about the N_2 ? Seems to me that observations here are treated like the holy grail but this is barely the truth when fitting and assigning errors.

- **The oxygen concentrations from WOA13 are in ml/l, its coverage is essentially shown in the figure (areas that are non-white) we have now altered to include the initial conditions of oxygen in ECCO and a scatterplot, and the ranges of point-wise values are shown in the scatterplot we now include. We use the annual climatology because $\kappa\rho$ in ECCO is not time-varying. If $\kappa\rho$ in ECCO were time-varying, then we would need to account for temporal variations in oxygen**

concentrations to evaluate the information they provide about $\kappa\rho$. N2 is a potential source of information as well, but this is tricky to compare with the model's N2 because of its vertical resolution compared to a typical observation's vertical resolution. Also, because N2 is determined from temperature, salinity, and pressure, that information may already be constraining $\kappa\rho$ in ECCO. These are the primary reasons why we didn't perform experiments with N2. We now include this sentence in the main text: "Due to the relatively coarse vertical resolution of ECCO compared with observations and the likelihood that information from N2 is already provided by temperature, salinity, and pressure, we do not directly compare N2 from ECCO with N2 from observations in another adjoint sensitivity experiment."

•125-130: Why the picture if you are outsourcing the most important thing to the Whalen 2015 reference? Just include the picture here for the sake of your readers. Also, This "justification" is not accompanied by a discussion of the methods/results. You need to explain in more detail what the insight here is and not outsource.

•I'm not sure if I understand this comment. The purpose of this figure is to show that there are similarities in the spatial distribution of vertical gradients in oxygen with the spatial distribution of $\kappa\rho$, W15. The correlation between the two products isn't strong, but a visual comparison of the two products suggests this is because the similarities in their spatial distributions is approximate. If there is non-local information in the oxygen data about $\kappa\rho$, then we could potentially see it through the adjoint sensitivity experiments we later perform in our study. This is supposed to help motivate our approach. We added the following sentence: "Any potential information that oxygen concentrations can provide about $\kappa\rho$ is likely through oxygen's vertical gradients because diapycnal mixing acts to erode water masses—which tend to be relatively homogenous in oxygen concentrations—along their peripheries." We also added the following sentence at the end of the ensuing paragraph: "Because of the possibly non-local relationship between $\partial O_2 / \partial z$ and $\kappa\rho$, we perform model experiments to further explore the potential information that oxygen concentrations provide about $\kappa\rho$."

•Figure 1. The justification at 125-130 is shallow and a bit out of place here that I wonder why the do/dz is the first figure in the paper. The first figure is an important milestone and the reason why this has to be do/dz is not fully commented - I don't think there is a backreference to this figure at all.

•We decided to add the Whalen et al. (2015) dissipation rates in this figure next to $\partial O_2/\partial z$ to show the spatial co-location of magnitudes more clearly. We also rewrote this entire subsection and now back-reference this figure later in the manuscript. This figure is one motivation (in addition to the arguments we make) for doing our simulations because the simulations can reveal whether oxygen concentrations provide information about k_p more clearly and convincingly than spatial correlations can.

•135-140: Humm objectives in methods? I think you could say that in the introduction and just explain what the model/assimiation is here.

•We have moved the two objectives to the last paragraph in the introduction.

•141: time-invariant but spatially varying K_p field? Show it - after all that is what you are trying to improve. Figure, figure, figure.

• κ_p is constant in time because ECCO is already solving an under-determined problem with all of the parameters and initial conditions it's estimating. We show in the Appendix that parameterizations in free-running models like KPP suggest it should be significantly time-varying in the subpolar North Atlantic in particular, but hardly anywhere else. We now include a figure of the depth-averaged (below the average mixed layer) of κ_p , ECCO.

•144: IMO table 2 provide enough details for the reader to clearly identify what the simulation is all about.

•We supplement this with a description in the main text to be certain that it's clear because other reviewers did not find Table 2 to suffice.

•150: What are the 14-day adjustments? this is the state estimate, right!? if so, say it here. All in all, Less model description, more framework description.

•The 14-day adjustments are parameter estimates that adjust the reanalysis forcing fields we began with. We clarified this issue with another reviewer as follows: the adjoint averages adjustments to the atmospheric forcing fields, which are re-estimated and then applied over 14-day periods. We have rephrased how we state this sentence: "Average adjustments to the wind stress, wind speed, specific humidity, shortwave downwelling radiation, and surface air temperature are re-estimated and then applied over 14-day periods."

•155-160: I miss a quick discussion about the K_p and your parametrisations. Why it is time-independent, caveats with the other parametrisations influences, and possible impacts and results (e.g. mixed-layer/convective adjustment and the oxygen results).

•We have edited the end of this paragraph to say the following: "Vertical mixing–diapycnal plus the vertical component of the along-isopycnal tensor–is determined according to the Gaspar et al. (1990) mixed layer turbulence closure, simple convective adjustment, and estimated background κ_p . Here, κ_p represents a combination of processes, including–but potentially not limited to–internal wave-induced mixing. κ_p , the Redi coefficient, and the Gent-McWilliams coefficient are time-independent because of the under-determined problem of inverting for initial conditions and model parameters would be even more under-determined if they were allowed to vary in time–explained below."

•170: So ECCO is fitting K_p and others already against other state variables. This should be at a table or in a more accessible location.

•The list of variables has been transformed into a table now. We include columns that indicate whether they're initial conditions or parameters, time-varying or time-independent, and two-dimensional or three-dimensional. Note that there are some variables that are time-independent and three-dimensional (only spatially-varying over each wet point) and other variables that are time-varying and three-dimensional (spatiotemporally-varying only over the surface).

•173: So you already start from an Optimized K_p - what about you starting from the 0 iteration with the data presented here? Also, what about the averaging done? The inner-loop is a whole year? Too so many gaps in information.

•I had to request the k_p field from the first iteration. One of my co-authors had this field available because he works with the people who did the optimization of ECCO. The k_p field from the final iteration is more publicly available. The k_p field is time-invariant so there's no temporal averaging.

•175-180: weak appendix link - you need to provide more material along the paper to entice the reader to read the appendix.

•We have included a reference to the first figure in the Appendix to justify why comparisons of κ_p from ECCO with κ_p from observations at particular times (e.g., from microstructure) and locations (in the subpolar North Atlantic) may not be appropriate. κ_p is likely to vary in time by about an order of magnitude over a year's time in the subpolar North Atlantic. Nowhere else does κ_p vary much, though, according to the model we use in the Appendix. The more relevant link with the Appendix in this manuscript is that sequential data assimilation systems have different issues with κ_p . These data assimilation systems can distort dynamical tracer fields because of their application of analysis increments, resulting in a violation of conservation principles. This potentially causes the model to undergo baroclinic adjustment, which can induce spurious vertical velocities and mixing. This isn't a problem in ECCO because only non-dynamically active fields are adjusted as the model is run forward and backward, and then the model is run over its entire time period length. In our adjoint sensitivity experiments, there is no adjustment in the control variables—only gradients are computed to inform how an optimization could be improved when we include new information in the cost function.

•I don't understand the -rerun here - you don't create a symbol for that and I can't see a reference anywhere. you are being repetitive here since you explain better in 190-195.

•The re-run is E-CTRL. The adjoint sensitivity experiments are E_k , E_O , and E_ε . We are more explicit about this in the bulletpoints, as you point out, but need to be clear that there are three types of simulations that can be done with ECCO in the application we're focusing on in our study: re-runs, adjoint sensitivity experiments, and optimization runs. We do not perform optimization runs here; the purpose of our study is to examine a potential motivation to do those more expensive simulations with observationally-derived k_p or oxygen concentrations.

•185-190: out of place - better around 150.

•Yes, we agree. We moved this passage.

•195-200: can you please define more formally what a forward ECOOv4 simulation is? a free run?

•Yes, the re-run is a free run, except it uses parameters that were estimated from the optimization. So the initial conditions and parameters (e.g., k_p and surface forcing fields) are inputs for the free run. We have added the following phrase to the text: "sometimes referred to as an ocean-only free run".

•No explanation previously of using N2 from WoA - I assume this is why you try to justify the $\partial O_2 / \partial z$ presented earlier right? This is badly connected.

•When we first examined the vertical gradients in relation to dissipation rates and κ_p from Argo floats, we now say: "The spatial correlation between $\partial O_2 / \partial z$ and κ_p , W15 is smaller in magnitude—about -0.1 —which motivates further consideration of the information provided by N2—derived from World Ocean Atlas (2013) temperature and salinity data with the TEOS-10 package (MacDougall and Barker, 2011)—later in this study."

• κ_p ECCO is 10^{-5} after optimisations or before? You said it was spatially vrying! κ_p ECCO is before or after state estimate!?! is κ_p ECCO from E-CTRL? You are not making the reader life's easier without naming simulations and parameters properly.

• κ_p is initially set to $10^{-5} \text{ m}^2 \text{ s}^{-1}$ before optimization. We show what the first iteration's estimate of κ_p (κ_p ,ECCO,0) and final iteration's estimate of κ_p (κ_p ,ECCO) are in comparison to microstructure. We also include a figure with a map of depth-averaged κ_p below the mixed layer from the final iteration. Each of these shows that κ_p ,ECCO is not $10^{-5} \text{ m}^2 \text{ s}^{-1}$ after optimization.

•210-215: Explain better why the results are independent of the run length. Is that just because you are using data in a climatological mode (averaging everything into a clim year!?). If you adjust fluxes and use observations, how the length doesn't count if by varying length you vary the amount of parameters to fit and such the Cost function?

•The results are not necessarily independent of the run length, but when we ran a longer simulation, we found similar results. This is likely due to our use of climatological fields for observations. We have clarified this by editing a sentence to say: "The adjoint sensitivities from Ek are not as sensitive to the run length as they are to the initial conditions of the run due to the lack of time-dependence of the observations included in the misfits- $\kappa\rho$ and oxygen concentrations."

•Your Eo starts from a different initial condition? Results in the methods? Sorry but this part is a bit of a mess - I think you should explain the sensitivity analysis and the assimilation before this part because this raises all types of questions (how the cost function is, background covar, B/R/Gain matrices, etc).

•Our simulations each begin from the same initial conditions. The only results we're presenting that had different initial conditions are the $\kappa\rho$, ECCO,0 profiles because the initial conditions estimated by ECCO after the first iteration are different from the initial conditions estimated by ECCO after the final iteration.

We now say: “We take the ECCOv4r3 solution as initial conditions for each of our simulations. We perform an adjoint calculation in each experiment, except for E-CTRL.”

•Figure2. This is a bit of out place and the reason why is not clear. The picture could show much more, such as the standard deviation of both model and obs. The colorbar got strange fonts, was this just pasted on the side. I would flick the centre of the picture (in fact all of them) to 180E picture to the pacific - since this is where errors are larger and where more data points are present (landmasses are distracting here). What is the depth of averaging? I would at least expect that you follow the 250-500/500-1000/1000-2000 you used in other figures so to give us something to reference regarding your results later.

•We now present a point-wise scatterplot to show the general agreement between the initial conditions for oxygen concentrations in ECCO and the oxygen concentrations from the World Ocean Atlas (2013). This includes every depth available in each data product. This should give the reader an idea of the standard deviations within each data product as well as the standard deviations of their disagreement. We also show the initial conditions for oxygen concentrations in ECCO for reference.

•225-230: I found the description here too simplistic and miss something more formal. This session falls apart without the apriori information. How the background error covariance is computed? Is it independent (apparently yes)!? What is the decorrelation length scale used? Several apriori facts are important here and the lack of these details are very concerning. How the setup and the equations are optimized/solved is nowhere to

be seen. This is the time to describe more fully how things work - so far all we got were sprinkles of incomplete information. Use a clear equation with the full state vector in each experiment. Is the 4dvar inner-loop a whole year?

•The ECCO framework does not use 4D-Var inner-loops because this mitigates the problem of non-linearity over long time scales; this is unique to the ECCO framework. But it sounds like you're referring to a sequential data assimilation system. We use the default decorrelation length scales for the smooth package in ECCO with the Weaver and Courtier (2001) method. This is explained in Forget et al. (2015). The smoother is applied to 1 grid cell in each direction, which means that the decorrelation length scales are $3 \times 100/e \approx 100$ km. Computing a background error covariance offline isn't necessary for our runs. The a-priori information in the model are climatologies that are documented in the ECCO literature. We are not excluding any information that is necessary to perform the adjoint sensitivity runs here.

•235: That 2% is optimistic. We need more details on how you declare the obs error. I think a lack of detail here is jarring and gives a bad indication/lack of attention on how the assimilation was setup. What is being corrected? Why you are not correcting Kp jointly with other observations? Just so your equations/W/J are simpler? If you don't use other state parameters in the equation, you are not using the full potential of the system (fitting the errors with T/S/SSH+Kp). I'm puzzled and can't see how these experiments are being conducted.

•The 2% comes from measurement errors for instruments commonly used to detect oxygen concentrations, which may be optimistic if we use an interpolated

observational product, but we are only including oxygen concentration observations where they were collected (at the nearest model grid point). Again, there is no "assimilation". It's just including these observations in a misfit to compute its gradients with the model's forward and adjoint matrices. We are considering only directions in the control space for how to improve k_p , given the optimization of the other variables. Of course the other control variables will be affected by the inclusion of a new variable like oxygen concentrations, but we did adjoint sensitivity experiments for these (e.g., Redi coefficients) and could not find more than about 50% agreement (random chance) between the adjoint sensitivities in an analogous pair of experiments to the ones we perform for k_p . This could be due to a lack of fidelity of the Cole et al. (2015)-derived Redi coefficient product or the fact that it's more strongly time-varying than k_p (below the mixed layer). In any case, we are examining whether there's motivation for an optimization run, not performing an optimization run ourselves, so the only variable that's influencing the control space solution is the new observational product. We have added the following sentence to the text: "We consider evaluating directions in the control space in which to improve k_p , given the values of the other control variables from the model's optimization."

•238: concerning K_p (and others).

•Thanks.

•240-245: What!? So you use model error/obs error as "sensitivity" for the K_p experiment? Explain why you decided to do this. I don't think you can use this equation - W is the solution - and you are imposing it? so you are just looking at the sign of "forecast

error" here and scaling it by the obs error!? Maybe using better wording or explaining better would remove the guesswork.

•We don't solve for W , but impose it based on the approximate measurement errors. We are trying to assess whether an observationally-derived quantity with a large uncertainty agrees (in direction of the control space) with an observation of a quantity with a small uncertainty. This is the simplest way to do it. The measurement uncertainties of other variables are used to determine their W so there's nothing different about this approach in ECCO. There is no "forecast" here.

•245-250: "Short of assimilating ... we assess whether the assimilation of a particular dataset *could lead* to a more ..." - !!! - This should be The first line in 225 - you are just confusing the reader - all of that text to say that you are just looking at the innovations and not performing it (apart from the Oxygen experiment I guess). I'm puzzled here about what is being done - you need to clarify the whole section 2. What you are optimizing here - W is usually the solution to the problem but you are imposing it now?

•We have moved this sentence to the beginning of the subsection. We are not optimizing anything with our simulations. We are simply comparing how k_p is being directed to change with new observational information included in the model's cost function, which could motivate a new optimization run with one of the observational data products included.

- 240-245: All that worry about K_p from different observations having different origins to just set the values like this? Also, the uncertainty here is related to the model to obs, not to obs to obs.

- In the ECCO framework, the uncertainty inversely scales with the weight for each observation and the uncertainty corresponds to observational uncertainty.**

- This part doesn't bode well for a robust setup in the sensitivity task. Also, there is no discussion about these settings and the sensitivity impact - you just let it for later I assume? (But this never happens down the results...)

- We discuss this in the results, where we mention the Monte Carlo simulations. We allow for uncertainties in the observed quantity and in the weights when we sample values of the adjoint sensitivities to get correlations between the sensitivities from different experiments. We now have a paragraph in this section that discusses this.**

•245-250: "Because the observations of Kp are not direct measurements...": Again nothing is a direct measurement (maybe Temperature is the closest thing), so this is not the reason to seek how the model Kp differ from observations...You just need to understand how the model errors are distributed in space/time. You just need to know how (γ -Sxtilde) looks like - just said it.

•We have changed the language here to no longer refer to in-situ observations as "directly measured" quantities.

•250-255: "However we dont want to assimilate ... because of their uncertainties and still limited spatial coverage relatively to oxygen". Why not? - because your constraint is only to Kp - you will be overfitting? Or because the equations you are using are not up to the Kp statistical log distribution? Why not try to solve the problem by assimilating Kp with all the other ECCOv34 parameters? This phrase here is probably locked in with the methods you are using so better to describe these insights with good information. Again some important concepts and insights are not being fully described here. I'm surprised by how this entire section confuses the reader.

•We are describing the analyses that need to be performed to determine whether it's a good idea to include observationally-derived kp products in the model's misfits and if it's unclear, then whether it's a good idea to include oxygen concentrations in the model's misfits. One of our conclusions is that either the uncertainties will be too large to place any constraint on the model's kp or the

resulting model-estimated $\kappa\rho$ won't be any more accurate than the observationally-derived products. It has been implemented in the model to use the log-transformed $\kappa\rho$ because of their distribution so that isn't a concern. We have changed the wording of this to: "We devote the first portion of our study to determining whether $|\kappa\rho_{\text{Argo}} - \kappa\rho_{\text{micro}}| < |\kappa\rho_{\text{ECCO}} - \kappa\rho_{\text{micro}}|$ (and, by extension, $\kappa\rho_{\text{CTD}}$ in place of $\kappa\rho_{\text{Argo}}$) is true. We do this because $\kappa\rho_{\text{micro}}$ is limited in its spatial coverage compared to $\kappa\rho_{\text{Argo}}$, $\kappa\rho_{\text{CTD}}$, and $\kappa\rho_{\text{tides}}$. Also, $\kappa\rho_{\text{Argo}}$ and $\kappa\rho_{\text{CTD}}$ are still limited spatial coverage relative to dissolved oxygen concentrations. While $\kappa\rho_{\text{tides}}$ has global spatial coverage, its measurement plus structural uncertainties are not well-known compared to dissolved oxygen concentrations..."

•256: I would assimilate both since they probably provide both information - but I'm not sure because you don't say what you are fitting here (boundary conditions? initial conditions? fluxes? model parametrizations?)

•One of our suggestions in the conclusions is that an observationally-derived $\kappa\rho$ should be used for $\kappa\rho_{\text{ECCO}}$ instead of including it in the model's misfits. This would reduce the number of parameters that need to be estimated in an under-determined estimation procedure and these observationally-derived products are closer to $\kappa\rho_{\text{micro}}$ than $\kappa\rho_{\text{ECCO}}$. It would still be possible to allow for some adjustments in $\kappa\rho$ if the observationally-derived products were assumed as a first guess within some uncertainty. Then oxygen concentrations could potentially help constrain $\kappa\rho$, if wanted.

•260-265: "is more than a factor of 3/ above". How this choice relates to the specified

errors in the fitting? No explanation and insight provided - seems a match-fixing kind of a problem when reading at first.

•There are reasons to do this. We need to be clear about this. Disagreements between the model and observational products in κ_p that are greater than a factor of 3 are outside the approximate uncertainty of the observational products; i.e., the differences are statistically significant. Also, regions where disagreements between the model's initial conditions and observations in oxygen concentrations that are within 2% are statistically insignificant. We are interested in where these both occur because these are regions where changes in κ_p are needed and the errors in oxygen are due to errors in the physics (e.g., κ_p), not initial conditions. We added this sentence: "We are interested in regions where κ_p is significantly erroneous and where the errors in oxygen are due to errors in the physics (e.g., κ_p), not initial conditions; hence, these choices."

•265- 270: I'm quite surprised by the lack of a discussion on how fitting for K_p will improve the model run since this is a parametrisation - the impact/practicalities and impact on dynamics are not discussed at all. The author refers that K_p is fixed in ECCO, but how is the model/analysis will perform after K_p is improved jointly or alone is left to the imagination. I understand now that the author is not looking for the analysis but just for the impact, but given the exoteric parameters, a mention of how this will flow down in the model run is important.

•Our paragraph regarding the motivation for using oxygen contains some of this discussion, but we now include some discussion of how an improved κ_p will

impact the state estimate. We added the following: "If $\kappa_{p,ECCO,0}$ is in closer agreement with κ_p from observational products than $\kappa_{p,ECCO}$, then errors in $\kappa_{p,ECCO}$ are likely being compensated by errors in other control variables beyond the first iteration of the model's optimization run. Inaccuracies in control variables can make physical inference using ECCO less grounded in reality and could make the state estimate itself less accurate—e.g., errors in κ_p will influence vertical tracer transport and mixed layer depths."

•270-280: More methods in results? "A geometric average is taken ...". New information about κ_p "log-normal". these need to be properly defined beforehand.

•We moved the methods-related sentence to the end of the paragraph describing the microstructure data in the methods section: "A geometric average is taken for each profile because this is more representative than an arithmetic average for a small sample size and when the data are not normally distributed (Manikandan, 2011), like the log-normal distribution of κ_p (Whalen, 2021)."

•284: not shown here? Really? The first result of the paper that can show some guess of spatial variability of K_p and you skip it!?

•We now show the spatial standard deviation of the $\kappa\rho$ profiles averaged over microstructure locations. We also show comparisons of $\kappa\rho$,ECCO,0, $\kappa\rho$,ECCO, and $\kappa\rho$,micro for 16 example campaigns. As mentioned earlier, we additionally show spatial variability of depth-averaged $\kappa\rho$,ECCO in a new figure. This is all in addition to the spatial variability shown in $\kappa\rho$,Argo and how it compares with $\kappa\rho$,ECCO and likewise for a new figure with $\kappa\rho$,tides.

•285: IMO, showing $K\rho$ vs $K\rho$, micro (Fig3) is better done after $K\rho$, W15. This is so because you show in Fig4 the locations of the microstructure which avoid the user to be distracted by Fig4 when reading Fig3.

•I had this order at one point, but other people who have seen this manuscript (including my co-authors) thought the order you saw made the most sense because the first result shown in this section should be a comparison with the gold standard measurement for $\kappa\rho$ and justification for trusting the Whalen et al. (2015) product (shown with magenta X's). However, now that we have a new, depth-averaged $\kappa\rho$,ECCO figure, we have moved the microstructure locations to this figure.

•Figure4. The right figures are misleading in regards to the other figures in the paper since white is not where data is missing, but where $k\rho$ = $k\rho$! I would recommend adding dot points where this situation was found to distinguish from the lack of data.

•Per another reviewer's comments, we have changed the colorbar to show a non-white color where the disagreements are small.

•kpargo is better than kpw15 reference, just as well kpctd is better than kpk17. Finally, I would help the reader here and say "that red(blue) areas are where argo is smaller (higher) than ECCO" since the log10 ratio.

•We have added the sentence, "Red (Blue) areas in Figs. 6b,d,f indicate locations where Argo-derived $\kappa_{p,W15}$ is smaller (larger) than $\kappa_{p,ECCO}$." We have also changed the notation for the different κ_p products derived from observations. Because we also include the de Lavergne et al. (2020) product, we refer to this product as $\kappa_{p,tides}$.

•295-300: I don't agree with how you define/use constraint here. Lack of agreement is not a lack of constraint. A realistic constraint is what? perfect match? the same order of magnitude? Define what you consider a good constraint or not. You can't in the paper because no one knows what is the initial K_p at all and how it was improved from the base case.

•We added the following text to the introduction: “Here, by ‘constrain,’ we were referring to using new data to change the level of agreement between the model and an observational product—not necessarily to achieve a perfect match.”

•300-305: This is just blaming without a proper discussion which should have happened beforehand to explain the limitations of the state estimate. Although I agree that compressing all the information required in a short text is a challenge, this ending appears a shoot in the foot - you can't give the reader proper insights of why k_p is not better constrained. You forgot to mention the numeric nature of the parametrisation and its limitations (plus the other parameters). Wouldn't be a leakage towards fixing the other parameters instead of k_p ? I miss some discussion around that.

•Per other reviewers' comments, we have added a discussion of how information from each observed quantity that is included in the misfit can change most—if not all—parameters. Oxygen concentrations would not be an exception. We focus on k_p here because there appears to be some correlation between the sensitivities of the misfits in oxygen and those in k_p . We investigated the sensitivities for another parameter— the Redi coefficient—and found virtually no correlation between the two types of simulations—50/50 agreement in sign. This doesn't rule out the possibility that the Redi coefficients—or other model parameters—would compensate for some errors in the way that k_p would change, though. Including information from more data sources could make this type of error compensation less prominent, though. We do not explicitly address this issue in our manuscript because we are not running optimization runs to examine this possibility. We are simply motivating the possibility of doing optimization runs that include oxygen concentrations.

•310-315: "Because $k_{p,ECCO}$ tends to be very large inside mixed layers" - another sprinkle of missing information in the middle. Couldn't you provide your readers with how $k_{p,ECCO}$ is beforehand?

•We have added a figure that shows $k_{p,ECCO}$ depth-averaged below the average model mixed layer. We exclude the mixed layer because k_p effectively doesn't do anything within a bulk mixed layer—it already being homogeneous in density. So k_p can be very large and the mixed layer will still be homogeneous in density.

•311-312: Another of saying it is "A positive adjoint sensitivity implies that the model overestimated K_p ". But isn't the k_p less than an order of magnitude compared to micro in Fig3? Globally, the tendency of your "adjoint" here is to increase K_p (more red than blue in Fig4), which is akin to what your GMAO results (appendix) are doing and overshooting the K_p beyond the microstructure. There is no discussion around this.

•A positive adjoint sensitivity implies that the model will reduce k_p because the objective is to reduce the misfit ($dJ < 0$) and the model determined that $dk_p < 0$. One takeaway from the combination of the microstructure-inferred and Argo-derived k_p comparisons with $k_{p,ECCO}$ is that $k_{p,ECCO}$ is too small compared with $k_{p,micro}$ and often too large compared with $k_{p,Argo}$. This is because the regions where microstructure measurements were taken tend to be in regions where $k_{p,ECCO}$ is too small compared with $k_{p,Argo}$. So the microstructure samples are not very representative of the entire ocean. We edited the last sentence of this paragraph to say: "Microstructure measurements tend to be regions where there are prominent topographic features and where the centers of subtropical gyres are found, which—judging from the predominant signs of disagreement in Figs. 4-5 versus Figs. 6b,d,f—aren't representative of the ocean

where Argo measurements were taken.”

•310-320: Why not a figure with adjoint sign profiles similar to Fig3? This would be more helpful than the whole description by region.

•The new figure we have with 16 example microstructure campaigns compared with $\kappa\rho,ECCO,0$ and $\kappa\rho,ECCO$ should help with this. Where $\kappa\rho,ECCO$ is too small (large), the adjoint sensitivities are negative (positive).

•Figure 5. Why not include a comparison of signals here? better than asking the reader to do that with these small figures and very gappy coverage. I'm also now presented that the calculations are done only for one year - 1992 - which is another surprise since this is not mentioned or discussed anywhere.

•Actually, this was mentioned on lines 208-209 of the version you read. The table quantifying the volume of the ocean over which the signs of the adjoint sensitivities agree from each experiment and the following figure get across the essential points we're trying to make. The purpose of the figure you're referring

to here is to present a visual comparison of how the adjoint sensitivities agree from each experiment.

•325-335: A global metric would be better here. Better metrics to compute %s would be beneficial in the paper since this is rather arbitrary. Maybe one or two regions of focus (one with a lot of obs - Kuroshio/North pacific and South Indian ocean?)

•**We quantify this in a table—both globally and regionally.**

•I found a bit daunting all the %s without a laser focus on the process at hand and where it will impact the most. The figures definitely need to be centred shifted towards the pacific.

•**We expect that oxygen will provide information about k_p away from regions with large air-sea flux of oxygen and away from the intensified jets. The subtropical North Atlantic Ocean is one region that previous studies have used oxygen concentrations to determine water mass erosion rates and residence times, and we find that this ocean basin has the highest percent agreement in**

the signs of the adjoint sensitivities across each experiment. The west Pacific is very different from the east Pacific in the quantities we show so we're not sure if centering the figures on the Pacific would help. We added the following to the first paragraph of this subsection: "We expect that the signs of sensitivities agree most in regions away from where air-sea fluxes and transport of oxygen—e.g., by intensified jets—are large. One of these regions is the subtropical North Atlantic Ocean, away from the Gulf Stream Extension."

•335-340: I think this deserves a new paragraph and more explanation since it is an important result.

•We have added the following sentence to this paragraph: "Thus, the regions with the largest disagreements in oxygen concentrations can always decrease their oxygen misfits by changing κ_p , ECCO with a sign consistent with decreasing its disagreement with observationally-derived κ_p ."

•340-345: Asking readers to calculate the white regions in one figure that are not white in the other !? tip: Making the life of the reader easier is the best way to make them happy. This is the most problematic aspect of using Fig5/Fig6 together since the white parts are misleading. You already set the reader mind that white is missing data, and now some figures perturb this notion and are used to reason about the results. I would refit Fig5/Fig6 to match the text and what you want to say more directly.

•We didn't ask the readers to calculate the amount of extra white area in one figure compared to another. We did the calculation ourselves and reported it. The rationale for the extra white area is as follows: we need to subset the data in order to control for the possibility that the bias in initial conditions is the reason for the errors in oxygen concentrations. We also are not interested in regions where k_p , ECCO is already consistent with observationally-derived estimates, within their approximate uncertainties. After we remove these possibilities that would confound our inferences, we are left with a little less than half of the comparable grid points.

•350:355: I would also wrap this in another paragraph since the insight here is important and related to the next paragraph at □360.

•We edited the first sentence of the paragraph near the line (we think) you're referring to: "Lastly, given that the general agreement in signs of sensitivities between E_k and E_O are likely underpinned by physical reasons unrelated to stratification, we pursue whether there is a statistically significant relationship between the adjoint sensitivities from E_k and E_O ."

•362: Finally a good insight, but not without trouble. You don't describe anywhere how N_2 is distributed, statistics, or where it will likely dominate against K_p and how it is related to it. Also, how this would be fit together with K_p (and other parameters) is a missing point

in the paper discussion.

•We now describe how N^2 is distributed, but already wrote several times how $\kappa\rho$ is related to ϵ through N^2 —because of the Osborn (1980) relation. We have added the following sentence: “ N^2 is generally about 10^{-7} – 10^{-5} s^{-2} , with lower values in high-latitude and deeper regions and higher values in the thermocline and in shallow water areas—which skew its global average (standard deviation) below the mixed layer to about 1.2×10^{-4} (3×10^{-3}) s^{-2} .”

•365-375: This end is badly written and looks like a last-minute addition. I would rewrite it since it is the concluding remarks.

•We have heavily revised this paragraph and split it into two.

•375-400: . I think it is too shallow here. There is no broad discussion of alternatives, cause/effects.

•We have heavily revised this whole section to discuss alternative approaches—i.e., not improving the agreement between $\kappa\rho$, ECCO and observationally- derived products but just using observationally-derived products to reduce the number of parameters the model estimates—and how to approach a new optimization that makes use of information from oxygen concentrations.

•390: Again the uncertainties are not discussed in terms of model error/background covariances/ inflation or decorrelations.

•Some of these issues are related to sequential data assimilation systems. The others we hope have clarified your concerns about uncertainties we did not discuss before.

•400-435: yes, yes, several things can affect but you don't discuss the real deal: fencing your results so people can locate themselves of what needs to be done next or how to relate this paper to their problem. IMO, at this stage, the reader is just tired of unlinked/big scoped caveats/problems instead of pin-pointed smaller scope discussion.

•We discuss the caveats, which are many-fold, but we also discuss what can be done to potentially improve the ECCO ocean state estimate, at least through improvement of $\kappa\rho$ now.

•440-eof : I will leave it to other reviewers/editors to see if this is important to be kept in the paper. Certainly, there are not enough references in the text to this section although some results are interesting from the point of view of assimilation. Also, important references in the appendix are not mentioned in the text and even some discussions related to the results presented are better than in the paper itself. Puzzling to understand why the author didn't include some of that in the actual sections!

•We now reference the Appendix in several locations in the main text. We didn't focus on the sequential data assimilation system results because of a computer crash where we lost much of the data and because we couldn't do justice to the cause of the large errors in $\kappa\rho$,GMAO, as I was never granted access to running the GMAO S2S data assimilation system (only what I could figure out on my own with the GEOS-5 model).