Review by van Heuven on the manuscript "Characteristics of Water Masses in the Atlantic Ocean based on GLODAPv2 data" by Mian Liu and Toste Tanhua

Liu and Tanhua present an enumeration of statistical properties of selected sets of seawater samples, thereby defining 'Source Water Types', likely for further use in Optimal Multiparameter analysis (OMPa) in a separate manuscript. Although of laudable intentions (having 'true' or 'universal' SWT definitions would make many a PhD student's life easier), I do not see why this paper should be published in its current shape – or at all.

My main criticism is, in increasing order of importance:

A) The ms. has not been carefully proofread, and glaring oversights remain.

B) Fundamental concepts in water mass analysis appear lost on the authors, rendering the findings of reduced usefulness for use by other investigators, who may work with a different conceptual framework of water mass analysis / OMPa.

C) The findings are trivial, and possibly not application-appropriate. (although I did not read the companion manuscript).

The large and rather thorough central portion of the manuscript may have merit as a review of literature on Atlantic oceanography – however I do not consider myself qualified to judge whether it may hold value over existing work in this regard.

I can imagine this entire paper to constitute, in severely condensed form, the first three paragraphs of a/the application paper. Almost all figures may then be moved to supmat.

Below, I'll list for each of the above categories — non-exhaustively —- some illustration to my criticism stated above, and provide further general commentary.

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*** A) "The ms. has not been carefully proofread, and glaring oversights remain".

Writing is worryingly sloppy. References are made to obviously wrong papers.

We examined the references carefully and corrected the misquoted references.

Abbreviations are jumbled.

We went through the manuscript carefully and corrected all the abbreviations to the right way of expression.

Example: – For GLODAP, reference is made to Lauvset et al (of the excellent mapped product). Given that the (bias-minimized) original bottle observations are used, reference should be to Olsen et al. That paper contains a fully self-contained explanation of the employed QC methods. This makes reference to Key et al., 2010 superfluous. Given the second authors exceedingly heavy involvement in these earlier publications, this slipup is surprising.

We read the methods section of Olsen et al., (2016 and 2019) carefully, and make changes in the description of QC part in the new manuscript (section 2.1).

Phrasing is occasionally imprecise and terminology (e.g., "variable", "value", "definition" etc.) is used inaccurately.

We unify the relevant expressions in the whole manuscript. For example: the word "**characteristics**" is used to describe the overall water mass (for example: characteristics of water masses); "**property**" is used to describe one special features such as oxygen (for example: six key properties); the word "**variable**" is not used in the relevant description in order to avoid confusion; "**value**" is used to show specific mathematical value; "**definition**" is used to show concrete concept.

Please carefully re-read. As an example: the caption to Table 1 now reads: "Table 1: Table of all the water masses and the four main layers as defined in this study. The variables defined are used to select water samples that defines water masses in the formation regions." but perhaps, much less ambiguously, should read: "Table 1: Summary of the criteria used to select (from GLODPAv2) the water samples considered to represent the source water types discerned in this study. For convenience, they are grouped into four depth layers."

Thank you for helping us out here with a clear linguistic organization. In the new manuscript, we now use clearer expressions to make the reader understand more easily.

*** B) "Fundamental concepts in water mass analysis appear lost on the authors, rendering the findings of reduced usefulness for use by other investigators, who may work with a different conceptual framework of water mass analysis / OMPa."

For instance, already the initial review section betrays a lack of understanding of the fundamentals of OMP. Line 67: "SWTs describe the original properties of water masses in their formation area, and can thus be considered as the original form of water masses (Tomczak, 1999)" is incomplete. For water masses defined as originating from a single SWT, this is correct. However, for WMs defined as being on the mixing line between two distinct SWTs (i.e., central waters), the statement is incorrect.

Thanks for pointing out the mistakes in our previous work. We read the reference (Tomczak, 1999) again, and indeed, Central Waters, which are formed by subduction through the thermocline and into the interior of the ocean, need to be treated differently from other deep water masses due to their different formation ways. In Section 3.0, this difference is pointed out.

Throughout the text, the terminology "SWT" and "Water Mass" is mixed up. The authors appear to not be aware of (or to subscribe to) the very specific, and non-identical, definitions of SWT and WM as provided by Tomczak 1999 (although that paper is cited).

A new section (Section 2.2) is added to distinguish the differences between "Water Mass" and "STW". In general, a "Water Mass" is an objective entity with temporal and spatial distribution; while a "STW" is a set of mathematical values that describes the original properties of a "Water Mass".

Rather, the terminology is used loosely, often incorrectly, and certainly confusingly. Tomczak states (paraphrasing) that "a water mass may be defined as either a point in parameter space, or as a line between two such points". All water masses discussed in the manuscript as treated as point sources, while in wider literature many (notably the Central waters) are generally considered to be "line sources". Please re-read Tomczak 1999 and follow its protocol. For highly relevant examples of what a hierarchy of water masses and their constituent water types could look like for the Atlantic, again, consider [Middag et al., ESPL 2018] or the chapter 7 of the thesis of Van Heuven, 2012.

Thanks for the guidance in distinguishing Central Waters and other deep masses.

In the revised version, we made amendments to this aspect. Central Waters are redefined as a line between two points, which are the upper and lower boundaries. In the Section 3.1, such distinction between Central Waters and other deeper SWTs is pointed out, and all the 6 key properties of Central Water, which cover relative larger ranges and cannot be consider as point values, are redefined by upper and lower boundaries.

In the figures (Fig. 4-7), all the data between upper and lower boundaries are plotted and the Central Water is still presented to the readers as one whole water mass. In the form of figure plots, Central Water has no difference to other deep water masses. The main difference is mainly reflected in the

OMP analysis, the central water masses occupy two "positions", which are the upper and lower boundaries and the values between them all considered as SWTs of this Central Water.

For example, in Section 3.1.1, the potential temperature (θ) of ENACW has clearly two boundaries. The upper and lower boundaries in potential temperature of ENACW are finally determined by the choice of our own fit ranges (https://omp.geomar.de/), 14.60 °C as the upper boundary and 9.80 °C as the lower boundary. All the other properties are done with the same method and the boundaries are listed in Table 3.

*** C) "The findings are trivial, and possibly not application-appropriate."

Effectively, the paper is an enumeration of means and standard deviations of properties of seawater samples encountered in (slightly arbitrarily drawn) multidimensional boxes in the ocean.

We agree with this assessment, and the intention of our work was not to redefine the water masses in the Atlantic Ocean, but rather to use the information already available and base the work on that. In several instances, water masses has in the past been differently defined and/or named so we tried to put this information in the paper as well.

Such defining of SWT properties would likely be re-performed by any investigator of Atlantic water masses. Presenting them here thus has little added value for the community. (exceptions may be long-term tracing of changing Atlantic water mass distributions, always employing the same SWT definitions. Such a ’climate change’ application though, would require a less subjective or circular approach to the defining).

The exact SWT definition used in a particular study may be very much application-dependent. E.g., where this study employs ’formations region’ SWT definitions, other studies (e.g., Middag et al., 2018) employ ’edge-of-section’ definitions for the water masses that have not been sampled at their formation regions. Other ’ad hoc’ definitions may be envisaged, and may be equally valid for the application at hand. That is, the definitions are subjective. Likely, for high-detail application, the results presented in this manuscript are too general. Conversely, for largest-scale application (i.e., basin-wide OMP), much more coarse approximations of the SWT’s may suffice (see for example Middag et al., EPSL 2018).

We disagree with this statement, at least partly. It is true that several investigators will go through the trouble to define their source water properties themselves, and possibly use “edge-of-section” data. We think that most do that since finding a stringent water mass definition is cumbersome. We provide in this work a comprehensive characterization of water mass properties that can be used by investigators. Obviously, the investigators focusing on a particular water mass might want to be more precise, and possibly look at temporal evolution etc. This paper is not intended for those, but rather for the chemical/biological oceanographers that would like to understand (roughly) the formation and mixing history of the water they sampled.

We explicitly aimed for being general and course in the WM characterization, realizing that “sub-water-masses” can be defined, and that spatiotemporal variability do exists.

*** Assorted commentary, in no specific order

– Although I’m a great fan of GLODAPv2, I do not see demonstrated that that data product is "uniquely ideal for use for SWT definition" (paraphrased from LINE 99), given its limited physical oceanographical detail. While GLODAPv2 is a very good biogeochemical data product, it features limited vertical resolution (vs. CTD), rather lax accuracy constraints for the exceedingly precise measurements of S and T. Without further corroboration of this statement, it is not evident why Gv2 should serve this purpose better than any other dataproduct that features S, T and O. Please elaborate. (Evidently, there may be additional value in having colocated values for N, P and Si, but I'd wager that will prove of little discriminating value for OMPa).

Point taken. I guess another products with biogeochemical data would do the work. The main advantages of Gv2 is the internal consistency of the data, so that we can use a large set of cruises and have some confidence that the data are consistent, which might be useful for water mass analysis. We do agree that high-resolution CTD profiles would be useful, for instance one can use potential vorticity as a parameter. Since our intended main audience are chemists and biologist with sparse vertical resolution of their data (mostly), this work corresponds to that need and the expected data availability.

– The CDW in the Weddell Sea, I believe is more commonly locally referred to as the "Warm Deep Water". It evidently does not include freezing waters. However, such samples are visible at 34.65/-1.9 in Figure 20 (likely located on the continental shelf of the Antarctic Peninsula). Please select more carefully – these skew your averages...

The selection criteria have been adjusted and data with low temperature (below 0 °C) are removed.

– Table 3: What is the use of stating "potential density" statistics (particularly for deep and bottom waters)? These would not likely be used for OMPa, because no information is contained additional to what is already contained in S and T. Also, they are formany SWT's pre-described through the sample selection criteria, so this is constitutes a rather circular result.

We agree, potential density is calculated from T and S, and is not an independent property of a water mass. The column of "potential density" is removed and Table 3 shows only 6 key properties of the water masses.

– Line 34: change "sea water type" to "source water type".

Changed.

– On conceptual grounds I have some trouble with referring to CDW as an SWT. Rather, it may be considered to be an aged mixture of the other SWTs presented. Large-scale (extended-)OMP-analysis that considers CDW will prove unusably under-constrained for samples from the CDW (i.e., such samples might be found to consist of 100% CDW, or of 33% of each of the other SWT, or any possible combination between). (However, OMP users may obviously choose to not include CDW an a candidate SWT). Same goes for "North East Atlantic Bottom Water". That water mass is not "formed" (F19 even mentions its "formation region"). It is merely AABW that flowed there, aging, and with admixture from (already defined) deep water. This is an intermediate to other more extreme STWs, that would already be accounted for in OMPa. Obviously, for a local study of, say, NE Atl. water masses, the NEABW SWT may be used, but please refrain from using "formation region" in its context.

Indeed, some water masses are not original water masses, but products of spreading and mixing, for example, NEABW. Because of their special properties and may be useful for region-specific studies, we hope to still keep such water masses and consider their SWTs. In terms of expression, we distinguish such water masses from ‘‘original’’ water masses, such as AAIW. We only show the key properties of such water masses in specific region, while the definition "formation area" is only for the ‘‘original’’ water masses. This is obviously somewhat subjective, but is introduced to facilitate the process of water mass analysis.

– Line 82: "our analysis is relatively course" ==> "coarse"

Changed into "coarse", new version in line 87

– I do not clearly see what the role is of the 4 density intervals discerned in this study? Are they merely to steer the reader's eye? Or are they used as additional boundaries to the vertical extent of selections of samples? Whatever the case, I believe that the two conceptually different ways of separating water masses by means of (i) OMP and (ii) density intervals are not necessarily compatible, and that these two methods should ideally not be mixed within a single paper, to avoid confusion.

The OMP method is the only criterion for distinguishing water masses in this study. However, there are a large number of water masses and OMP analysis can only calculate no more than 6 water masses within one OMP run (with the number of variables we have to our disposal). Therefore, the ocean is divided into 4 layers according to the density (in total 13 OMP runs, divided by density and latitude as shown in the following table) that to ensure no more than 6 water masses are present in each OMP run. Therefore, density can also be considered as an additional boundary, which will be further clarified in this article so as not to confuse the readers.

50°S Equator 40°N

#13 AAIW AABW CDW WSBW	**#6** WSACW ESACW AAIW	**#5** WSACW WNACW ESACW ENACW AAIW	**#1** WNACW ENACW SAIW MOW
(σ_θ = 27 kg/m^3)	**#8** ESACW AAIW uNADW	**#7** ENACW ESACW AAIW MOW uNADW	**#2** ENACW SAIW MOW LSW
(σ_θ = 27.7 kg/m^3)	**#10** AAIW uNADW lNADW CDW AABW	**#9** AAIW MOW uNADW lNADW NEABW	**#3** SAIW LSW ISOW DSOW NEABW
(σ_θ = 27.88 kg/m^3)	**#12** lNADW AABW	**#11** lNADW NEABW	**#4** ISOW DSOW NEABW

– Line 120: "for some SWTs, key properties such as salinity, oxygen or silicate are also necessary". It may warrant some discussion as to why this does not constitute circular reasoning. For example, if one pre-defines the S-range for the samples, then the resultant average S is of little intrinsic value! This is pertinent for example to the definition of MOW ("36.35-36.65"), which in reality has salinities well beyond the statedrange.

The criteria in Table 1 are listed according to historical literatures. Based on these criteria, we selected eligible data from the GLODAP dataset, and then make statistics on these eligible data to obtain a result (gaussian distribution), and these results (or values) are considered as the basis for our definition of SWT. Therefore, besides the area distribution (latitude, longitude and depth), it is also necessary to list some criteria in Table1, because there may be other water masses in the designated area, and we need to use these criteria to eliminate the interference of external water masses. But, that being said, it is a somewhat circular argument that we define the range of a variable (e.g. S) for the definition of the water mass, and then use that to estimate the average value of that variable. However, it serves to use well-known characteristics of water mass properties to define them also in this paper.

– Most (panels of most) figures should be moved into supmat. Please maintain only an interesting subset of figures for the main ms.

This is a good point. We do think that the figures are an important part of the paper. Now, particularly since we have merged the two manuscripts into one, we do have an exceedingly large number of Figures. We will carefully make a selection to which figures will be moved to supmat. Thanks for the suggestion.

– Figure 1 – this cruise is not drawn in on the map. Consider plotting it in F2. You can't expect readers to google the cruise track themselves.

A small figure (map) is added to show the cruise.

– Figure 22: no characters in circles in legend. I believe it to be a shame that the paper does NOT present alternative property-property presentations of the definitions derived. Possibly, nothing beats a set of theta_vs_x plots (or similar) for visualizing the multidimensional separation of the various SWTs. For inspiration, please refer to, for instance, figure 7.5 in the thesis of van Heuven (2012). Also, from F22 I recon that there's some extremes of the samples in the S-T diagram that are not accounted for by any watertype. For example, in F22, panel B, the few hundred (?) samples at -1/34.9 have no closely associated SWT. These samples – while indeed part of the Atlantic Gv2 – are located in the Norwegian Sea, which is not covered in your work. Remove these from the figures to improve legibility and aid understanding. Also, many hundreds of samples are located at salinities well below that of AAIW (several standard deviation of the AAIW SWT definition). Are these surface samples? If not, how would these ever be represented accurately in an OMPa? For an example fix, please consider the SWT definitions in figure 7.5 of van Heuven (2012).

We have made corresponding modifications and adjustments to the figure as suggested.

– Line 128 "[...] the standard deviation of the distribution (the amplitude of the curve defined as 2/3 of the highest bar)". This does not ring a bell as being a definition of standard deviation. Please rephrase.

Description is reorganized, in new manuscript line 228.