



Centennial persistence of subantarctic water mass anomalies after a reversal of CO₂ forcing

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Abstract. We use machine learning analysis to classify subantarctic water masses and explore the centennial-timescale persistence of their anomalies under idealized atmospheric CO₂ ramp-up and ramp-down simulations in a general circulation model. Our definitions of individually labelled water masses are not based on fixed density and temperature ranges, arbitrary thresholds, or many of the other subjective choices that may not be universally applicable across observations and models, but only on the ocean layers' relative differences in stratification, salinity, temperature, and density. These novel flexible definitions adapt under the anomalous warming, freshening or salinification, lightening, and increased stratification of the water masses in simulations forced with an increase followed by a decline in the atmospheric CO₂ concentration after a 2°C or a 4°C global warming peak. Without such flexible water mass definitions, analysis of ocean layers would suggest an apparent depletion or even disappearance of some water masses in a warming world. Under emission scenarios with a higher peak warming, intermediate waters and Lower Circumpolar Deep Water decrease in volume, while the volumes of Subantarctic Mode Water (SAMW) remains approximately the same, and the reservoir of accumulated Antarctic Bottom Water (AABW) shows a local expansion. The flexibility of our machine-learning approach allows us to study the persistence of subantarctic ocean anomalies on centennial timescales as global warming is subsequently reversed. Subantarctic Mode Water shows freshening that becomes persistent on centennial timescales after a +4°C global warming peak. Intermediate and Circumpolar Deep Waters also show persistent freshening on these timescales, while Antarctic Bottom Water exhibits centennially persistent salinification both after a +2°C and a +4°C global warming peak. The slowest rates of recovery of temperature and density as CO₂ concentrations decline are seen in the deep ocean layers mixed with North Atlantic source waters. In terms of magnitude, the largest temperature anomalies that persist once the CO₂ concentration is returned to preindustrial values are seen in the subtropical waters and in Upper Circumpolar Deep Water. Across subantarctic water masses, the temperature and volume anomalies that arise for warming of up to +4°C do not recover on centennial timescales when negative CO₂ emissions are imposed. The anomalous warming of Circumpolar Deep Water and Antarctic Bottom Water exhibits persistence even after a +2°C global warming peak.



1 Introduction

The Southern Ocean plays an important role in the climate system as a sink of anthropogenic carbon and anthropogenically induced heat anomalies (Sabine et al., 2004; Sarmiento et al., 2004; Gao et al., 2018; Williams et al., 2024). The Subantarctic Mode Water (SAMW) and Antarctic Intermediate Water (AAIW) store a particularly large amount of anthropogenic carbon (Sabine et al., 2004) and heat (Armour et al., 2016) at depth. The SAMW layer impacts both the long-term anthropogenic trends and the variability in the ocean heat, carbon, and oxygen budgets. For example, Gao et al., (2018) show that a thickening of the SAMW layer constitutes the dominant contribution to the 2005-2015 increase in upper ocean heat content south of 30° S. Older southern water masses such as Circumpolar Deep Water (CDW), which contain North Atlantic Deep Water (NADW) as a major source, carry a large concentration of natural carbon that can be outgassed from the Southern Ocean to the atmosphere (Olivier and Haumann, 2025). The deepest water mass, Antarctic Bottom Water (AABW), which is denser than CDW, stores a substantial fraction of the global ocean heat anomaly and contributes to as much as 9% of the thermal expansion component of present day global sea-level rise (Purkey and Johnson, 2010). In this study, we focus on the magnitude and persistence of thermodynamic changes in the subantarctic water masses.

Traditionally, water masses are defined in density space with bounds corresponding to potential density surfaces, neutral density surfaces, or approximations to neutral density surfaces (e.g., Johnson, 2008; Sallée et al. 2013; Abernathey et al, 2016; Fu et al., 2024; Kostov et al., 2024) under the assumption that these closely match material surfaces. Such density-space frameworks allow the computation of surface transformation rates (Speer and Tziperman, 1992; Abernathey et al, 2016; Desbruyères et al., 2019; Kostov et al., 2023; Fu et al., 2024) and more comprehensive layer volume budgets following the classical Walin (1982) approach. Relative differences in vertical stratification (or its contribution to potential vorticity) and salinity can help distinguish individual water masses (Sallée et al. 2013; Boland et al., 2021; Kostov et al., 2024; Pimm et al., 2024).

Sallée et al. (2013) introduce an extension of the traditional water mass definitions that is more universally applicable across observations, preindustrial and historical simulations with various models, as well as future scenarios and projections. The Sallée et al. (2013) approach puts the emphasis on identifying local extrema in stratification and salinity as a starting point for labelling water masses in density space without assuming that a given individual water mass must be found on the same specified density layer across observations and diverse model simulations.

We build upon the pioneering work of Sallée et al. (2013) by introducing a machine-learning algorithm to identify water masses based on local extrema in vertical stratification and salinity superimposed on spatially varying potential temperature and potential density. Compared to the analysis of Sallée et al. (2013), our approach leaves even less room for arbitrary choices when defining water mass criteria. The latter emerge in an unsupervised manner as we cluster Southern Hemisphere ocean data points from model simulations under various CO₂ emission scenarios. Random forest models (Lanham et al., 2026) and Gaussian Mixture Models (Oglethorpe et al., 2026) have been used in previous studies for identifying the fractional contributions of water masses sources. However, as we wish to define ocean layers with bounded



volumes and finite heat content values, in our study we use a k-means clustering (Hartigan, 1975) algorithm for the unsupervised classification of ocean data points into water masses. Following this approach, we label each water parcel as belonging to only one water mass at any point in time.

70 With our water mass identification framework, we can explore the persistence of subantarctic water mass changes on centennial timescales in response to an increase and then a decline in greenhouse gas forcing. In our study, an ensemble of idealized atmospheric CO₂ overshoot simulations with the coupled atmosphere-ocean-ice sheet and sea-ice UK Earth System Model (UKESM) allows us to analyse the transient behaviour of the important subantarctic water masses and the reversibility or otherwise of their warming and lightening induced by greenhouse gases (Smith et al., 2026).

75 There are various definitions of tipping points, regime shifts, and irreversibility in the climate literature (Ridley et al., 2012; Arellano-Nava et al., 2025; Winkelmann et al., 2025). Here, we adopt a practically-oriented rather than a mathematically derived approach towards reversibility and consider persistence encompassing both long-term inertia and true hysteresis behaviour of the ocean (Smith et al., 2026). We therefore refer to such behaviour as “centennial-timescale persistence,” as both our prescribed forcing and the adjustment of the subantarctic ocean response evolve on a timescale of centuries.

80 Our clustering algorithm identifies water masses based on their “functional” differences in relation to one another. As the world warms under simulated CO₂ emissions, the water mass properties change but the differences between adjacent water masses stay qualitatively similar. Thus our approach presents a novel perspective on the evolution of southern water masses under greenhouse gas forcing.

85 In Section 2 we describe the model configuration that we use and the simulation protocol, as well as the clustering algorithm we apply for identifying water masses in our domain of interest. In Section 3 we present results from the model’s preindustrial climatology and simulations forced with atmospheric CO₂ emissions. We probe the persistence of water mass changes under ramp-up and ramp-down of atmospheric CO₂. In Section 4 we discuss the implications and limitations of our findings.

2 Methods

90 2.1 Model

We use output from simulations conducted with UKESM1.2, a version of the CMIP-class Earth System Model updated from previous versions described in Mulcahy et al. (2023) and Sellar et al. (2019) by the addition of two-way coupled Greenland and Antarctic ice sheet components (Smith et al. 2021; Siahayan et al., 2022; Smith et al. 2026; Naughten et al., 2026). The icesheet domain is represented by BISICLES, a dynamical ice sheet model (Cornford et al., 2015), and the atmospheric 95 domain uses the Unified Model atmosphere component version 3.1 (Kuhlbrodt et al., 2018; Williams et al., 2018). The ocean component is the G07 eORCA1 version of NEMO3.6 (Storkey et al., 2018; Madec et al., 2017) with an equivalent 1° resolution, 75 z-coordinate vertical levels and a representation of the ocean domain under floating Antarctic ice shelves.



Interactive icebergs are included in the ocean domain (Marsh et al., 2015) and sea-ice is represented by the CICE model (Hunke et al., 2015). Previous studies have shown that UKESM reproduces the climate and water masses of the Southern Ocean well compared to modern observations despite the relatively low spatial resolution (Smith et al. 2021; Siahaan et al. 2022, Gomez-Valdivia et al. 2023; Naughten et al., 2026). We refer readers to the listed references for a more complete description of the components of UKESM1 and how they are coupled together.

2.2 Simulation Protocol

The simulations used in this study follow the idealised TIPMIP-ESM protocol (Jones et al., 2025) in which warming and cooling are forced by the imposition of artificial fluxes of carbon dioxide. The simulations start from a quasi-equilibrium preindustrial baseline in which the model's carbon sources and sinks have been spun up to be in balance so that global mean atmospheric CO₂ does not drift. The climate is first warmed using a constant emission rate of 8 Gt CO₂/yr, an amount that has been calibrated to produce a warming rate of global mean surface air temperature (GMSAT) of approximately 2°C/century in UKESM. The TIPMIP-ESM ensemble of simulations contains multiple CO₂ ramp-up realisations. However, only one of the available ramp-up experiments (cx209) is ultimately branched and sub-branched into CO₂ ramp-down simulations. This is the ramp-up ensemble member that we use in our analysis. It represents the UKESM realisation of TIPMIP experiment up2p0, here called the “ramp-up.” Two further simulations are branched from the ramp-up. When GMSAT reaches 2degC above the preindustrial baseline, CO₂ emissions are reduced to 0 GtCO₂/yr for 50 years, and then become negative at -8 GtCO₂/yr cooling the climate back to the preindustrial GMSAT; this branch is TIPMIP up2p0-gwl2p0 followed by up2p0-gwl2p0-50y-dn2p0, here called “2K ramp-down”. A similar zero- and negative-emission branch is created when the ramp-up reaches a GMSAT of 4degC above preindustrial which we call the “4K ramp-down” (TIPMIP up2p0-gwl4p0 followed by up2p0-gwl4p0-50y-dn2p0). For context, an overview of the polar climate, ice sheet and sea-ice response in UKESM1.2 following this protocol is presented by Smith et al. (2026).

2.3 K-means clustering of ocean data points into water masses

In our study, we identify subantarctic water masses using the K-means clustering algorithm (Hartigan, 1975), an unsupervised machine learning technique that can efficiently classify large and multidimensional data points into groups characterized by relatively similar properties. This approach has been successfully applied in oceanographic studies of water masses (e.g., Sun et al., 2021; Jin et al., 2023; Romero et al., 2024). Other machine learning techniques such as random forest models (Lanham et al., 2026) and Gaussian Mixture Models (Oglethorpe et al., 2026) have also been used for identifying source water fractions. However, unlike the aforementioned methods, the k-means clustering algorithm has the advantage that it draws sharp boundaries between ocean layers corresponding to individual unique water masses. This allows us to define water mass budgets for temperature, salinity, density, volume, and heat content.

Our choice of ocean properties for determining the clustering is based on the approach for water mass classification put forward by Sallée et al. (2013). The latter demonstrate a robust methodology for defining water masses consistently



130 across observations, different models, as well as historical simulations and future projections. Instead of imposing fixed
potential or neutral density bounds or characteristic temperature and salinity ranges, they consider the local minima and
maxima in potential vorticity (PV), salinity, and temperature across multiple density layers in the Southern Ocean. Sallée et
al. (2013) define some of the water mass boundaries in terms of density ranges centred on the local minima and maxima in
salinity. We take their approach further as the k-means clustering algorithm allows us to eliminate the so-called “arbitrary
135 constants” remaining in the Sallée et al. (2013) algorithm: their imposed distances in density space relative to the salinity and
PV extrema, and the constants used to specify PV thresholds in the water mass definitions. Instead, our k-means clustering
lets the water mass classification emerge in an unsupervised manner from the relative “proximity” of different ocean data
points.

Here we apply the k-means algorithm to Southern Hemisphere ocean data between 40°S and 60°S from a set of
140 UKESM PI control, CO2 ramp-up, stabilisation, and two CO2 ramp-down simulations (a 2K a 4K ramp-down). We choose
this latitude range because it encompasses important subantarctic water masses that are found at the gateway to the Southern
Ocean and that play a first order role in the global heat and carbon budgets under greenhouse gas forcing. We stop at 60°S
because further south, especially in the sub-ice shelf cavities, we would need to account for additional precursors to and
modified varieties of the water masses that we analyse in our domain. For example, further south, we would encounter
145 modified versions of Circumpolar Deep Water, as well as different regional varieties of shelf water and bottom water that
contribute to the formation and northward export of Antarctic Bottom Water.

Each ocean data point in the domain of interest is characterised by four dimensions: potential temperature [°C],
salinity [psu], potential density referenced to a depth of 4 km [kg m⁻³], and potential vorticity (PV) [m⁻¹s⁻¹]. PV is
approximated as proportional to the planetary vorticity captured by the Coriolis parameter f and, crucially, the vertical
150 stratification of the ocean captured by the buoyancy frequency N :

$$|PV| \approx \left| f \frac{N^2}{g} \right|. \quad (1)$$

Vertical stratification or potential vorticity is an important criterion for distinguishing water masses (Sallée et al., 2013).
However, In the winter and early spring, the near-surface stratification decreases substantially across all density classes,
which renders the PV criterion less easily applicable for distinguishing water masses in these seasons. We aim to draw
155 distinctions between the different water masses as they have different regions of formation and destruction, and different
evolutions of their properties, volumes, and heat content in a warming world. That is why we choose to focus only on April
months, corresponding to the beginning of southern hemisphere autumn, when volumes of high and low stratified water are
found at depth in isolation from the shallow low-stratified mixed layer. April marks the beginning of each new seasonal
cycle of local convective formation or destruction, import or export, restratification, and local accumulation of water
160 masses. In order to leave out the early autumn mixed layer, we only look at water masses below 200 m. Selecting only April
has the limitation that we do not explore the months when some of the southern water masses under consideration are formed
locally at the surface, but we rather focus on what remains of these water masses after each cycle of formation, destruction,



import, export, and storage at depth. This means that we look at the net accumulation of water masses over the seasonal cycle instead of isolating variability in the surface formation and transformation of water, processes which are marked by the exchange of heat and carbon between the ocean and the atmosphere. In addition, by selecting April months and depths below 200 m, we leave Antarctic Surface Water (AASW) and Winter Water (WW) out of our analysis for the in the present study.

Before applying the clustering algorithm, we compute the z-score of the data set along each of the dimensions, i.e., the number of standard deviations relative to the mean along each dimension. This converts distances to unitless standardised measures. Admittedly, there is an inherent arbitrary choice underlying this conversion. Namely, there is an implicit assumption that all distances in potential temperature, potential density, salinity, and PV space are treated equally in terms of their respected standard deviations instead of giving a greater relative weight to one of these dimensions, e.g., salinity, for defining water masses. These abstract dimensions of potential temperature, potential density, salinity, and PV are not orthogonal to each other. In our April water columns below 200 m, the ocean is thermally stratified and hence, temperature and density covary very strongly. It is worth reiterating that we use potential temperature referenced to the surface but potential density referenced to a depth of 4 km. Even though these dimensions are correlated, referencing one to the upper ocean interface, and the other one to the deep ocean allows us to simultaneously apply the algorithm across a range of vertical levels.

Fixing the number of clusters in the k-means algorithm is an additional arbitrary user-defined choice. However, we approach this decision using both physical and mathematical arguments. First, we consider the variability of water mass properties in density space, as illustrated by meridional sections in the Southern Hemisphere April pre-industrial control climatology (Fig. 1). Overall, as we go from lighter to denser layers (or as we go north to south in the horizontal direction in the April climatological sections between 40°S and 60°S), we see two local maxima and two local minima in PV magnitude (Fig. 1b). There are also two maxima and two minima in salinity in density space, visually identifiable in meridional sections (Fig. 1a). However, the salinity and PV extrema are not aligned with each other, allowing us to identify the fingerprints of 7 water masses that can readily be labelled using conventional names. Both Subtropical Mode Water (labelled at 35°S in Fig. 1) and Subantarctic Mode Water (labelled at 42°S in Fig. 1) are local minima in the magnitude of potential vorticity, but Subtropical Mode Water is a local maximum in salinity, while SAMW is marked by low-salinity. In fact, in this UKESM configuration, SAMW rather than the more highly stratified Antarctic Intermediate Water (AAIW, labelled along 47°S in Fig. 1) is the salinity minimum in this latitude range. This differs from observations, where AAIW exhibits the lowest salinity (Sallée et al., 2013). Nevertheless, in this UKESM configuration, the highly stratified AAIW is still marked by very low salinity comparable to the adjacent SAMW (Fig. 1). The next two water masses, Upper and Lower Circumpolar Deep Water (UCDW and LCDW) are both more saline than the adjacent AAIW. The low stratified LCDW (labelled along 57°S in Fig. 1) spans a local salinity maximum, as expected. Poleward and deeper than the LCDW salinity maximum lies the less-stratified and fresher AABW. Normally, a local minimum in oxygen concentration would help identify UCDW (Callahan, 1972). However, due to a bias in this UKESM configuration, the oxygen minimum is not found in UCDW but rather in layers denser than the LCDW salinity maximum (not shown).

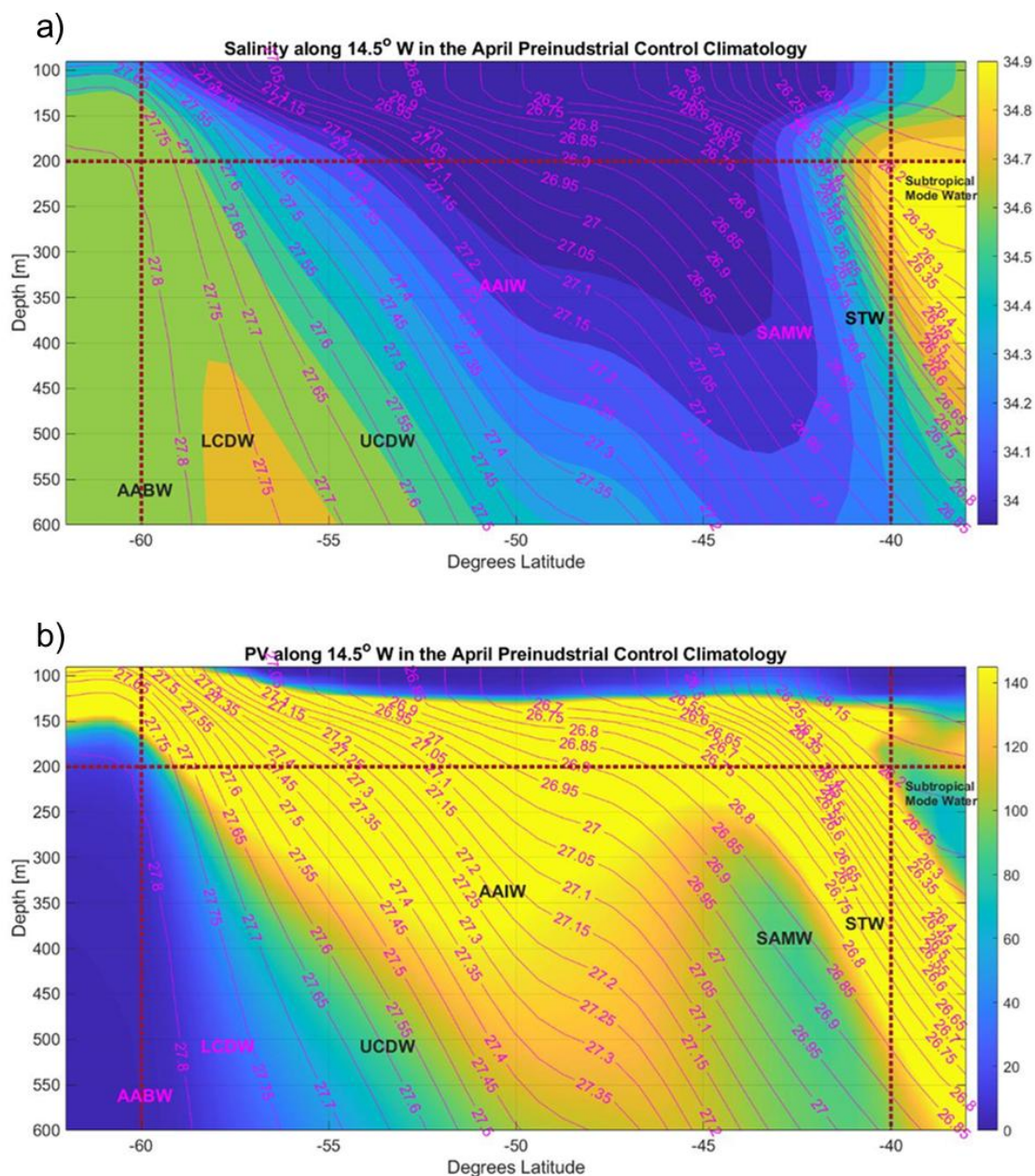
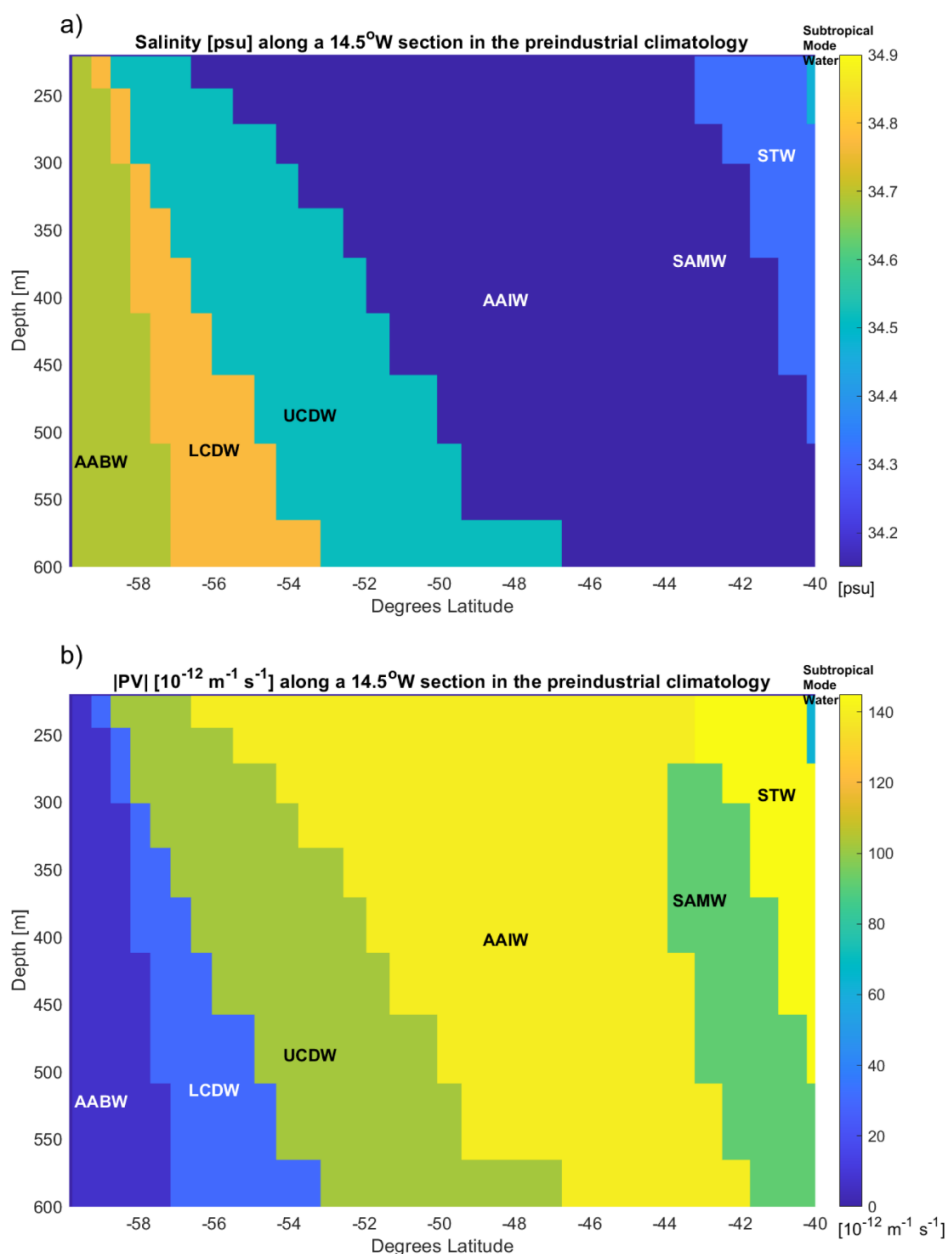


Figure 1: Climatological meridional sections of top: salinity [psu] ; bottom: magnitude of the $|PV|$ [$\text{m}^{-1}\text{s}^{-1}$]. Superimposed are σ_θ contours [kg m^{-3}]. Individual water masses are labelled with conventional names by visual inspection (e.g., the local salinity maximum corresponding to LCDW).



205 **Figure 2:** Same as Fig. 1 but showing the properties of the clusters in the April pre-industrial climatology. Top: salinity [psu]; Bottom: PV [10⁻¹² m⁻¹ s⁻¹]. Properties of each cluster centroid are remapped over the entire cluster volume in space and then a section along 14.5°W is selected. Notice that here we show only the region between 40°S and 60°S below 200 m, corresponding to the box partially delimited with dotted lines in Fig. 1.



210 Furthermore, especially in the Atlantic Sector, the larger temperature contrast between SAMW and Subtropical Mode Water leads to a sharper highly-stratified thermocline barrier between them, that we label Subtropical Thermocline Water (STW), adding up to seven water masses (Fig. 1) in our region of interest. This relatively thinner highly-stratified layer appears to be absent in the April preindustrial climatology of the Indo-Pacific sector. In this sector, we find Subtropical Mode Water adjacent to SAMW. This is consistent with the notion that Subtropical Mode Water is a primary contribution to
 215 the formation of Indo-Pacific SAMW (Fernández Castro et al., 2025), whereas SAMW in the Atlantic is largely advected from the Southeast Pacific. Our qualitative initial examination of these ocean sections thus gives a physical motivation for imposing 7 clusters in our k-means algorithm.

We furthermore test how the classification changes as we vary the number of clusters applied to the preindustrial control climatology in the region and depth range of interest. To that end, we use the so-called gap value criterion that
 220 imposes a trade-off between the skill of classifying points into clusters and the number of assumed clusters (Appendix A). We vary the number of clusters k , and apply the k-means algorithm to our preindustrial control climatology, where each time the first guess for the cluster centroids is randomly initialized. We see that the gap statistic increases with cluster number k . However, with $k=7$ clusters, we obtain a statistic whose value exceeds 67% of the projected gap statistic for the hypothetical case of hundreds of clusters (Fig. A1a in the Appendix). In addition, the marginal improvement in the gap statistic is much
 225 larger for cluster numbers lower than 7 compared to $k>7$, and there is a noticeable drop in marginal skill gain at $k=7$ (Fig. A1b in the Appendix). The mathematical quantitative analysis of the clustering skill thus matches our physically intuitive judgement that we can qualitatively identify seven water masses by traditional approaches.

A standard approach towards initializing the k-means clustering algorithm is to use randomly generated cluster centroids as a first guess before iteratively optimizing the clusters and their centroids. We use this randomized approach
 230 when we explore the gap value criterion for different values of k , as described above. However, in our main scientific analysis of the UKESM simulations, we initialize the cluster centroids with non-random values as follows. We start our analysis by clustering the April preindustrial climatological data using initial guesses for the cluster centroids (Table B1) based on typical water mass core potential temperature and practical salinity properties in previous observational and model intercomparison studies (e.g., Johnson, 2008; Sallée et al., 2013). There are no firmly established core temperature and
 235 salinity properties of the highly stratified Subtropical Thermocline Water in literature, and for that we use a qualitative first guess based on a visual inspection of the preindustrial April climatology (see Table B1). Potential temperature and salinity are used to compute σ_4 potential density as an additional cluster property, assuming a reference pressure level of 4 km. Using potential temperature referenced to the surface but potential density referenced to the deep ocean allows us to diversify the clustering criteria, so that we can apply one and the same algorithm from the surface all the way to the ocean bottom and
 240 capture both upper ocean water masses and AABW. In the initialisation, we furthermore assume relatively low magnitude PV for Subtropical Mode Water, SAMW, and LCDW ($-75 \times 10^{-12} m^{-1} s^{-1}$), a relatively higher magnitude of PV for STW and AAIW ($-100 \times 10^{-12} m^{-1} s^{-1}$), and almost zero stratification for AABW ($-0.10 \times 10^{-12} m^{-1} s^{-1}$), where these PV initialization values (Table B1) are idealized round numbers rather than attempts at exact guesses. After the initialisation, the



algorithm is then allowed to iteratively optimise the cluster centroids to better match the data points from the model simulation.

After the k-means algorithm identifies the optimal cluster centroids and boundaries for the model’s preindustrial April climatology, we use the resulting cluster centroid positions to initialize a k-means algorithm for April in Year 201 of the PI control run (a year that is long after the initialisation of the control simulation but more than a century before the branching of the CO₂ ramp-up). The resulting clusters are our labelled water masses in that year, and their centroid properties are used to initialize the clustering algorithm for April in the following year, Year 201. Once we have a history of at least 20 years, we always use the clustering results averaged over the preceding 20 years as our first guess for initializing the algorithm in the following year of the PI simulation. Averaging over two decades to obtain the initial guess for each year has the advantage that we reduce the numerical noise in the clustering and capture the gradual evolution of the cluster centroids under CO₂ forcing. In contrast, randomly initialising the cluster centroids gives rise to noisy and difficult to interpret results when the algorithm is applied to simulations with an increase and a decrease in CO₂.

When the CO₂ ramp-up is branched from the PI control, we continue applying the clustering each April and using the result of the preceding 20 years as a first guess for the k-means algorithm applied the following year. The same approach is analogously applied when analysing the stabilization and ramp-down simulations.

We do not feed depth, latitude, and longitude data into the clustering algorithm, and we process the ocean datasets as long vectors without any representation of the 3-dimensional spatial structure of the ocean fields. However, the data points in each cluster correspond to actual ocean grid cells in the model that can then be labeled as belonging to one water mass or another and remapped onto their respective latitude-longitude-depth spatial coordinates. We do not use any spatial smoothing to post-process the resulting output. In addition, even though we use σ_4 in our clustering algorithm, we furthermore compute the cluster potential density referenced to other depths: σ_θ and σ_2 . These re-mappings of the results in depth and density space allow for a better physical interpretation.

After applying the algorithm, we obtain the mean potential temperature, potential density, and salinity for each water mass, as it evolves in time, in addition to a well-defined volume of each water mass in the domain of interest. Knowing the potential temperature θ and the layer volume V then allows us to calculate the time-evolving heat content anomaly $\mathcal{H}$ in each water mass k in our domain, relative to the initial preindustrial heat content. In our case, we use a reference based on the initial heat content in the year when the CO₂ ramp-up simulation is branched from the PI control experiment and express the heat content anomaly $\mathcal{H}$ as:

$$\mathcal{H}(k, t) = \rho_0 c_w V(k, t) \theta(k, t) - \rho_0 c_w V(k, 0) \theta(k, 0), \quad (2)$$

where $\rho_0 = 1026 \text{ kg m}^{-3}$ is the reference density and $c_w = 3991 \text{ J kg}^{-1} \text{ K}^{-1}$ is the specific heat capacity of sea water, and t denotes time after branching from the PI control simulation.



275 3 Results

3.1 Potential temperature, potential density, salinity, and PV

In our classification of the water masses in the UKESM PI control April months, the 7 clusters that emerge are marked by a monotonic decrease in temperature (and increase in density) from the subtropics to the deep waters of North Atlantic and polar origin (Fig. 2 and 3), similar to what is apparent in a visual inspection of model sections (Compare Fig. 1 and Fig. 2).
 280 Superimposed on these monotonic gradients is the presence of the minima in PV magnitude (Fig. 3) that can also be matched to the local minima in PV magnitude found in Subtropical Mode Water and SAMW in the meridional sections (Fig. 1 and Fig. 2). AABW stands out as a low-stratified (low PV magnitude) water mass fresher than LCDW and denser than the local salinity maximum in LCDW (Fig. 1 and Fig. 2).

The clustering also identifies a local salinity minimum spanning both SAMW and AAIW (Fig. 3), which is different
 285 from the assumption of Sallée et al. (2013) that the salinity minimum can be used to strictly define AAIW. In fact, in some years of the PI simulation, the absolute April salinity minimum is found in the low stratified SAMW rather than in the more highly stratified AAIW (Fig. 3), although, overall, the two water masses retain salinity values similar to each other from one year to another. This wide SAMW-AAIW salinity minimum may be a model-dependent feature of our particular configuration, which would make the Sallée et al. (2013) algorithm less appropriate for identifying AAIW in our PI
 290 simulation, and suggests that their approach is not universally applicable.

Spatially, the horizontal and vertical fingerprints of the water masses emerging from the clustering algorithm of the PI simulation are physically meaningful and interpretable as aligned with the major oceanic fronts in the region (Fig. 4, Fig. C2 and a description of the front identification in Appendix C) and distinguishable ocean layers that outcrop in the sub-Antarctic Southern Ocean. For example, in the horizontal fingerprint and in the vertical sections, we can identify SAMW and
 295 AAIW layers that extend farther north in the Atlantic Sector compared to the Pacific, as expected from observations (Fig. 4).

In addition, we find that in the Indo-Pacific sector, Subtropical Mode Water is in direct contact with SAMW, while in the Atlantic Sector, the two mode waters are separated by a thin layer of highly thermally stratified water (Fig. 4, 5). The same basin asymmetry is found when comparing meridional sections in the Atlantic and Indo-Pacific Sectors (Fig. 5). There are indications that under CO₂-induced warming, the highly stratified barrier between SAMW and Subtropical Mode Water
 300 can strengthen in particular hot spots in the Pacific (e.g., along 150°W), but this does not appear to be a signal stronger than natural interannual variability in the PI control simulation (not shown).

An important result that is achieved by the clustering algorithm is its ability to identify the same “functional” water masses even under very strong global warming of +4°C (Fig. 4, 5). For example, our clustering recovers the dynamical boundary between southward flowing LCDW, the adjacent northward flowing AABW layer in potential density space at
 305 $\sigma_2 \approx 37 \text{ kg m}^{-3}$ (Fig. 6 and 7), which shows as a minimum in the density-space overturning streamfunction.

To a first order, under increased CO₂ forcing, the water masses present in the PI simulation retain the same horizontal and vertical fingerprints and approximately the same three-dimensional locations, yet they warm and lighten (Fig.



4, 5). We find that under the ramp-up, all water masses lighten, and all of them except subtropical waters become more stratified, attaining higher PV magnitudes (Fig. 8), and a positive stratification anomaly, which implies a reduction in the ocean's ability to take up heat and carbon at depth and to maintain the inventory of dissolved oxygen (Oschlies et al., 2018; Sallée et al., 2021). In some cases, under strong warming, a given layer becomes as light as its neighboring layer initially was in the PI simulation, yet such large trends pose no challenge to our algorithm. Even though the water mass properties change quantitatively, their comparative relationships relative to adjacent water masses remain qualitatively the same.

Relative PV and salinity extrema remain in approximately the same geographical locations under CO₂ ramp-up as in the PI simulation and in the same water masses identified by our clustering (Fig. 3, 4, and 5). Except for several outlier data points, the algorithm results show that the LCDW cluster remains the most saline cluster, more saline than the adjacent AABW cluster despite the salinification of the latter (Fig. 9). Our LCDW tracks very well the temporal evolution of the deep salinity maximum in density space (Fig. 10).

Although our clustering algorithm exhibits occasional numerical noise in the cluster salinities (the sporadic excursions in Fig. 9), we can still draw physically meaningful conclusions. Among the water masses explored in our analysis, AABW and Subtropical Mode Water exhibit salinification under CO₂ ramp-up (Fig. 9). The salinification of Subtropical Mode Water appears to persist both after a +2°C and a +4°C global warming (Fig. 11). In contrast, AABW does not return to its lower preindustrial salinity when CO₂ concentrations are lowered below preindustrial values (Fig. 11) after a +2°C global warming.

Our surprising result showing a salinification of the AABW cluster under a CO₂ ramp-up is in fact matched by a similarly evolving salinification trend when we consider the most low-stratified ($|PV| < 10^{-11} m^{-1} s^{-1}$) water near the bottom (Fig. 12). The lightening of the AABW cluster also approximates the magnitude and evolution of potential density of the most low-stratified ($|PV| < 10^{-11} m^{-1} s^{-1}$) water near the bottom (Fig. 12).

The salinification of Subtropical Mode Water and AABW can be contrasted against the freshening of AAIW and SAMW in the simulated warming world (Fig. 9 and 11). The freshening anomaly in SAMW reverses when CO₂ is lowered after a +2°C global warming, but persists (exceeding 0.2 psu of freshening) if CO₂ is ramped down after a +4°C global warming peak (Fig. 11). In comparison, AAIW shows persistent freshening exceeding a reduction in salinity irrespective of whether CO₂ is ramped-down after a +2°C or a +4°C peak (Fig. 11). The persistent freshening anomaly in AAIW is ≈ -0.1 psu after a ramp-down to PI concentrations following +2°C warming and a ≈ -0.2 psu following after +4°C warming.

Under CO₂ ramp-up, UCDW and LCDW show prolonged freshening, which eventually slows down (Fig. 9). LCDW salinity exhibits nonlinear behaviour. The gradual freshening giving way to salinification under very high global warming rates beyond +4° (Fig. 9, 13). However, when CO₂ concentrations are lowered right after a +2°C or +4°C global warming peak, the freshening anomaly in LCDW persists (Fig. 11).

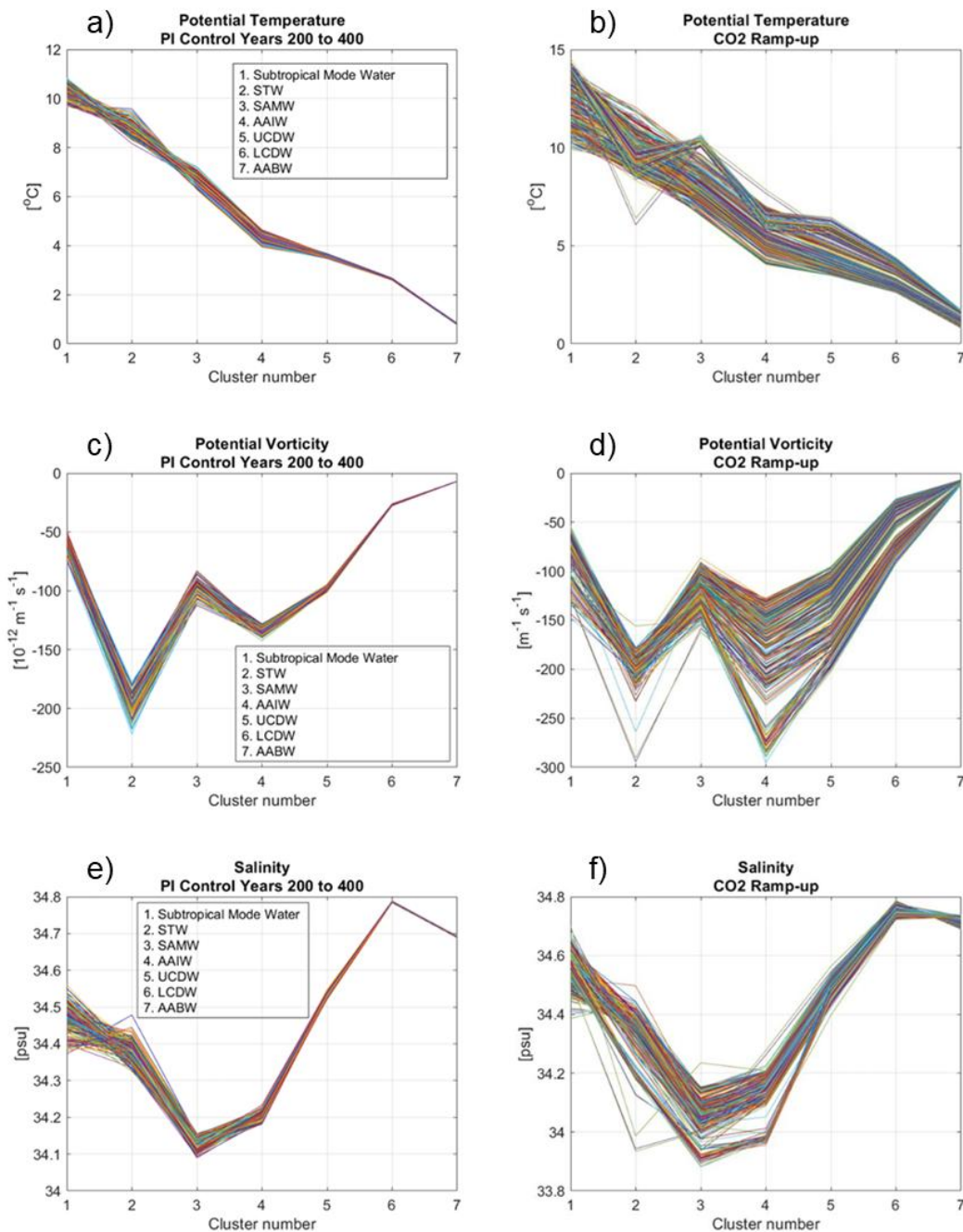


Figure 3: Left, centroids in the PI climatology: potential temperature [$^{\circ}\text{C}$], PV [$\text{m}^{-1}\text{s}^{-1}$], salinity [psu]. The horizontal axis indicates the cluster number, which corresponds to a given water mass. Each coloured line in a given panel represents the clustering in a given month of April between Years 201 and 400 in the PI Control. Right: Same but for the CO2 ramp-up. Notice that Cluster 2 (STW) is not a well-defined volume of water; it has similar properties to SAMW but is marked by a high PV magnitude (high stratification).

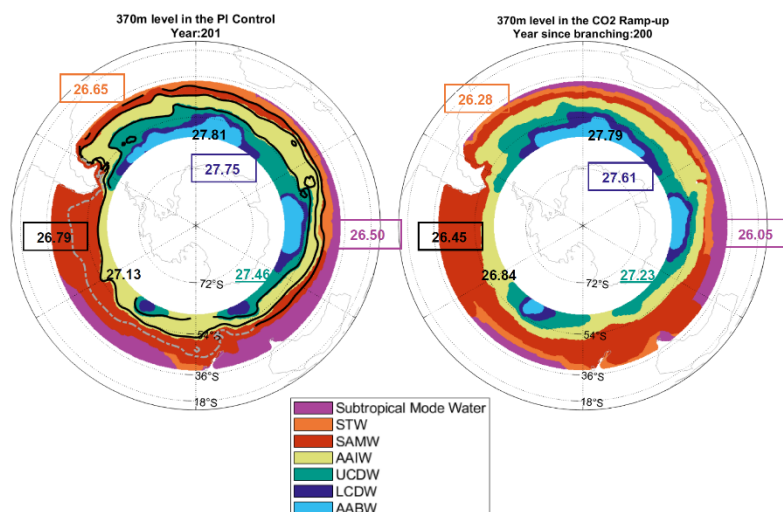


Figure 4: Horizontal sections at a depth of 300 m. The left shows an April average in Year 201 of the PI control. Superimposed are the horizontal locations of the Subtropical Front (STF), the Subantarctic Front (SAF), and the Polar Front (PF). The STF is shown only in the Indian and Atlantic Sectors (see Appendix C). The right shows an April average 200 Years into the CO2 ramp-up, once a global warming average of +4°C is reached. Text in boxes indicates the σ_θ potential density [kg m^{-3}]. Individual colours from the accessible colour scheme [Tol, 2021] correspond to different water masses.

The persistent salinification of AABW and the freshening of LCDW (Fig. 11) are ultimately related. As the climate warms, the supply of new AABW precursors shuts down and the deep overturning cell south of 55°S disappears (Fig. 7). At the same time, as the AMOC declines (Fig. 7), both the import of LCDW precursors and the northward export of AABW weaken substantially (Fig. 7). As a result, between 40°S and 60°S, we are left with old reservoirs of LCDW, AABW, and their respective precursors that mix with each other without being resupplied sufficiently. Thus, the old reservoirs exchange salinity (Fig. 9 and 11) and the salinity gradient between them weakens (Fig. 3) under a CO2 ramp-up. This is consistent with the results of Gunn et al. (2026), who find a long-term salinification of AABW.

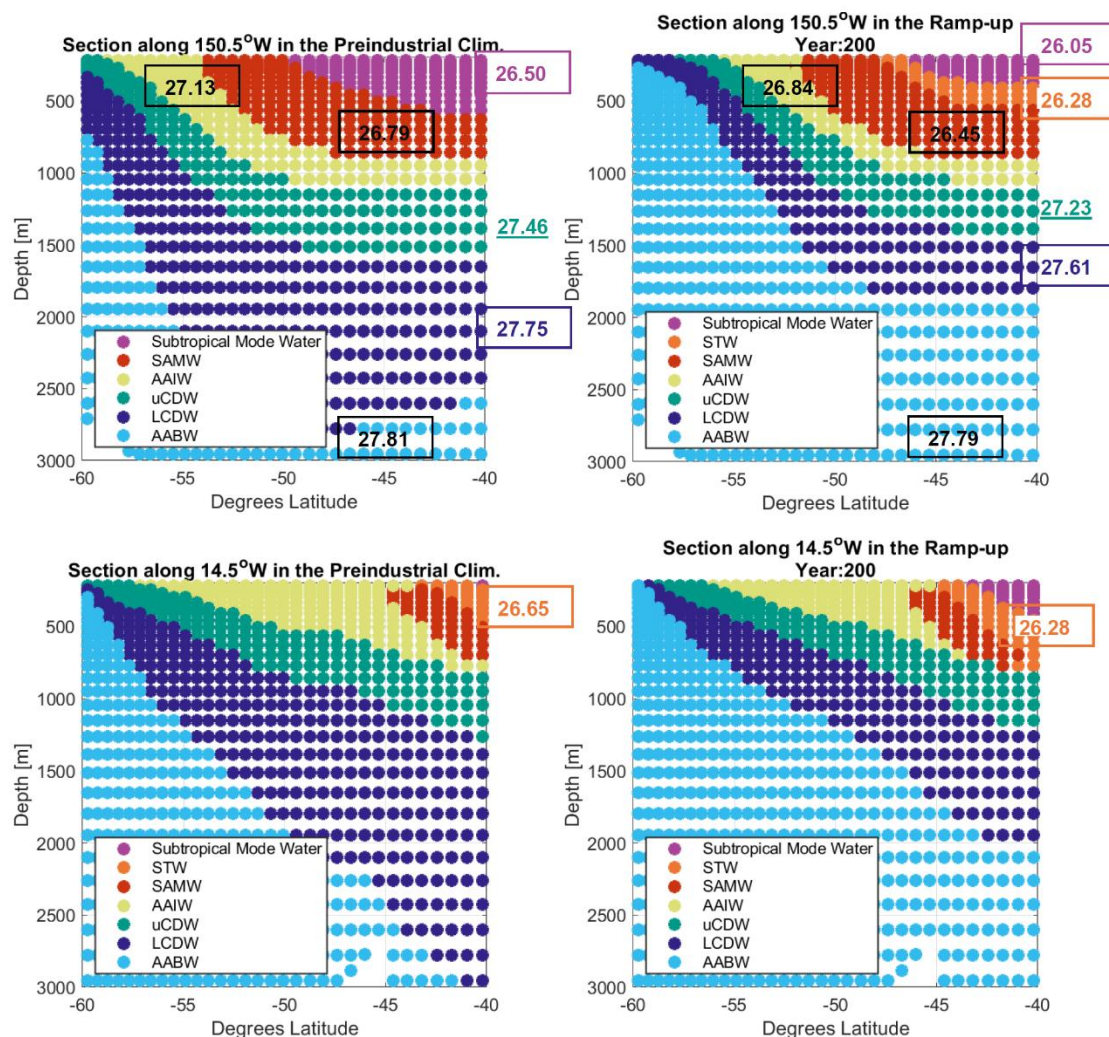


Figure 5: Same as Fig. 4 but with meridional sections along 150.5°W (top) and along 14.5°W (bottom). The left column shows an April average in Year 201 of the PI control. The right column shows an April average 200 Years into the CO₂ ramp-up, once a global warming average of +4°C is reached. Text in boxes indicates the σ_θ potential density [kg m^{-3}].

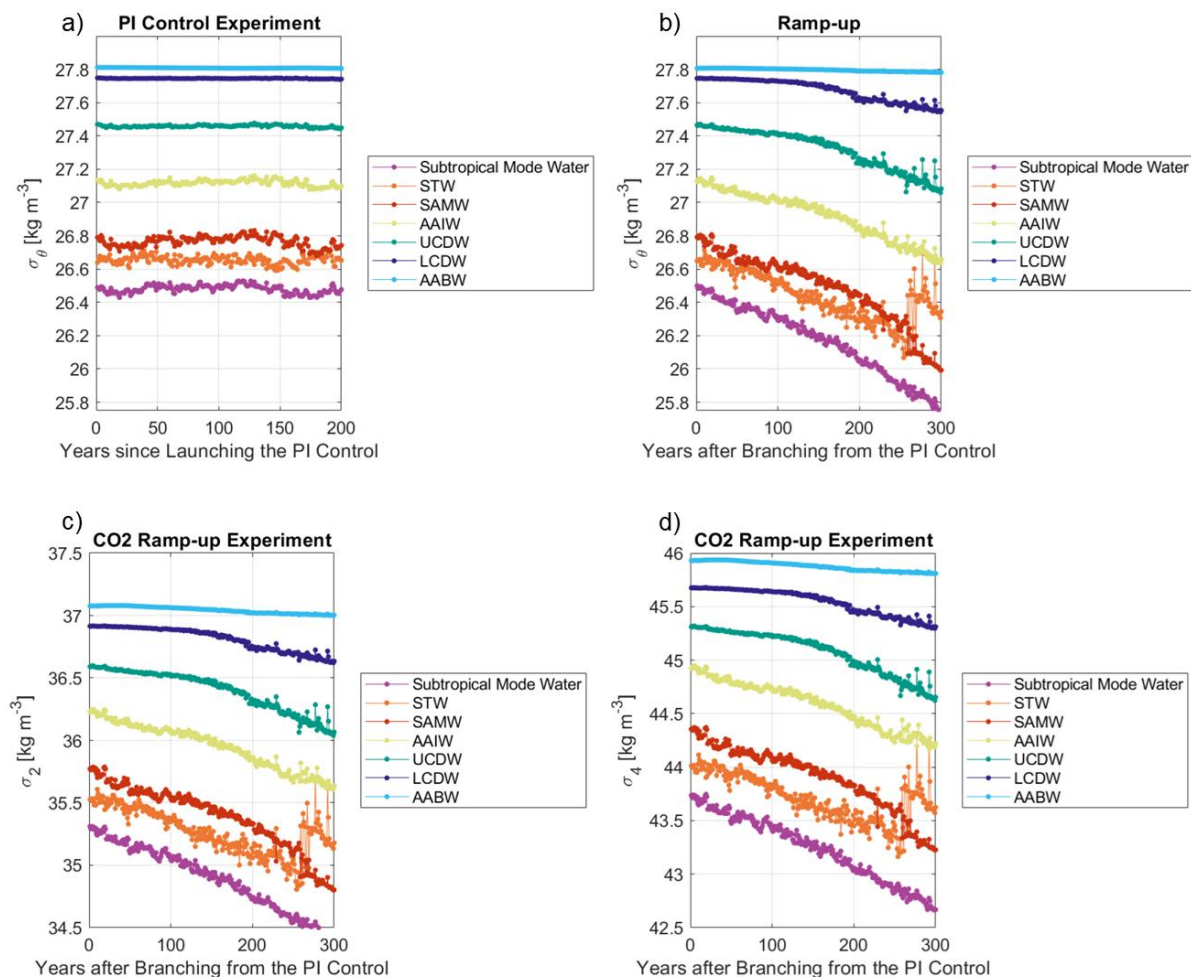


Figure 6: Temporal evolution of potential density referenced to the surface in the PI control (top left) and CO2 ramp-up experiments (top right). Bottom row: similar but for the evolution of potential density referenced to 2 km (left) and 4 km (right) in the CO2 ramp-up experiment. Notice that STW is not a uniform water mass but encompasses all parcels that are similar to SAMW, yet highly stratified. Later in the ramp-up, STW separates not only SAMW from Subtropical Mode Water, but also SAMW from the denser AAIW (Appendix D).

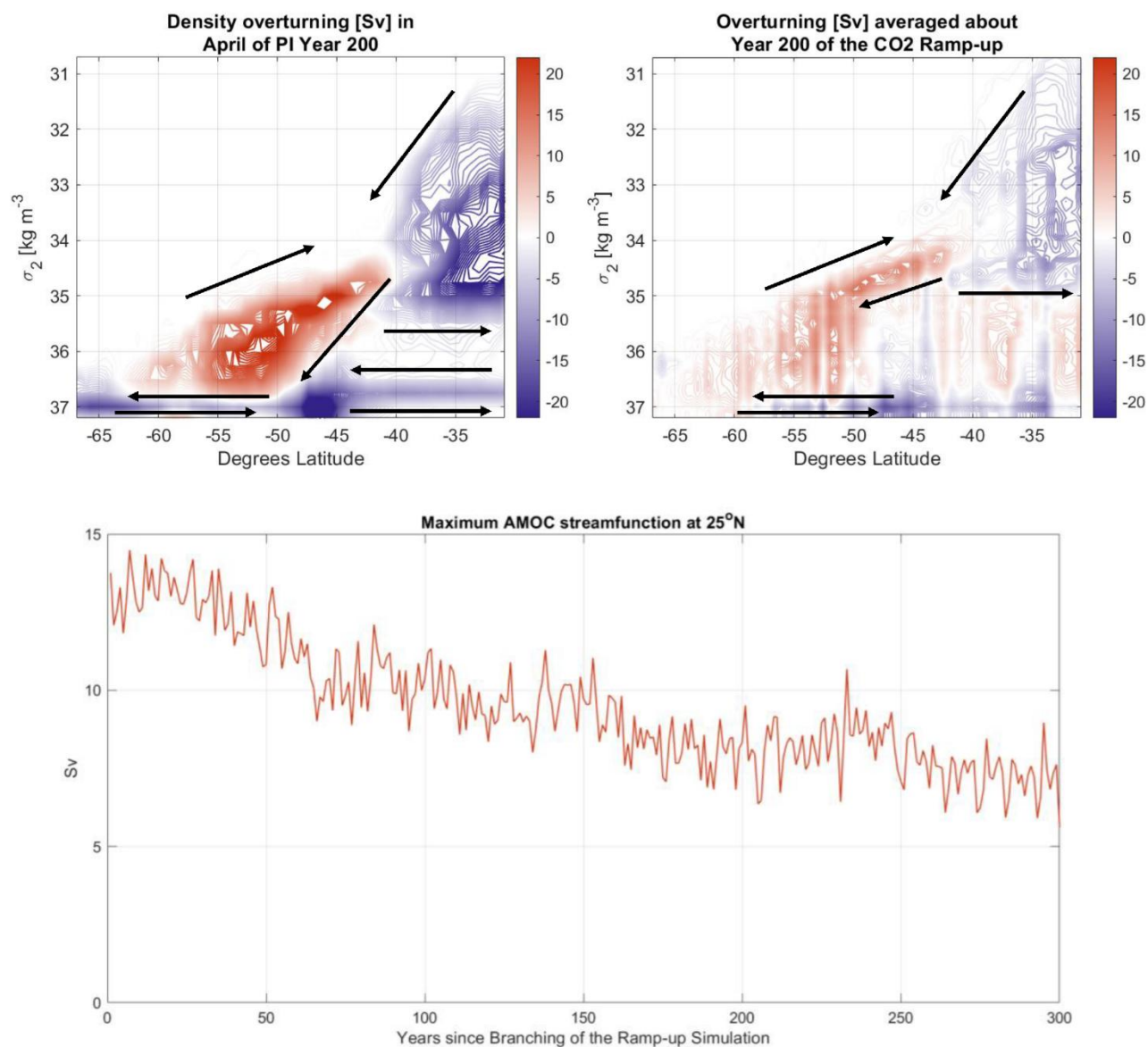


Figure 7: Top: Global meridional overturning streamfunction in σ_2 potential density space (referenced to a depth of 2 km) in the PI control (a) and in a 20-year mean centered on Year 201 of the CO2 Ramp-up (b). Positive values and red shading indicate clockwise overturning and blue shading indicates counterclockwise flow in the figure, as additionally indicated by black arrows. Bottom: (c) the Atlantic Meridional Overturning Circulation (AMOC) streamfunction maximum in depth space at 25°N.

In addition, some of the identified watermasses in our region show persistent enhanced stratification under a CO2 ramp-up (Fig. 9). For AAIW, UCDW, and LCDW, this increased magnitude of the PV persists after CO2 concentrations are reduced after a +2°C or a +4°C global warming peak alike, while for AAIW, the noticeable persistence in stratification (a PV magnitude anomaly $\approx 40 \times 10^{-12} \text{m}^{-1} \text{s}^{-1}$) is seen after a +4°C global warming peak (Fig. 11).

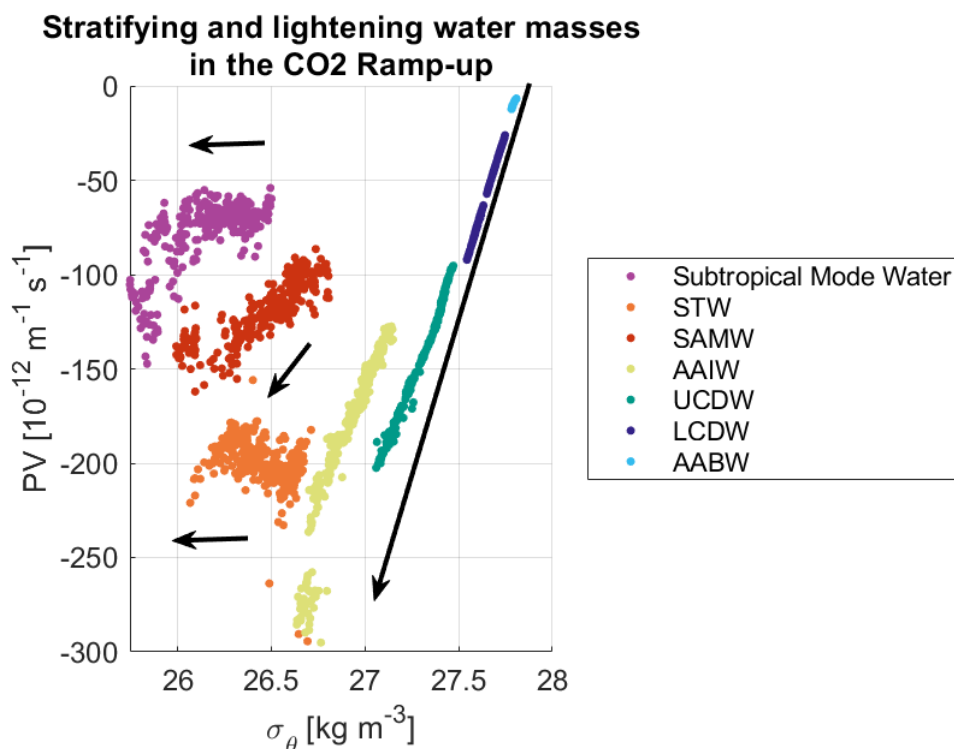


Figure 8: Increased stratification and densification of individually clustered water masses throughout the course of the CO₂ ramp-up experiment. Each marker indicates a cluster centroid in a given month of April during the ramp-up. Schematic arrows denote the direction of temporal evolution.

Interestingly, SAMW experiences a qualitative shift to high stratification after a +4°C global warming (Fig. 8 and Appendix D). Under warm conditions, part of the SAMW layer becomes very strongly stratified and difficult to distinguish as belonging to the local minimum in the PV magnitude. In this situation, the remaining low-stratified SAMW becomes a water mass with a different spatial fingerprint, no longer a continuous circum-Antarctic band of low stratification, but rather a set of patches that are spatially isolated from each other or punctured by areas of very high stratification (Fig. D1). This qualitative change is state dependent. It is not seen if the peak warming is limited to approximately +2°C. This regime shift appears after a +4°C global anomaly both in the ramp-up, and during a CO₂ ramp-down from +4°C, as the subantarctic region marked by high thermal inertia continues to warm. Because this qualitative change emerges both in the extension of the ramp-up simulation to higher temperatures above +4°C and in a ramp-down of CO₂ after a +4°C global warming peak (Fig. D1), we suggest that the new SAMW regime is a robust feature.

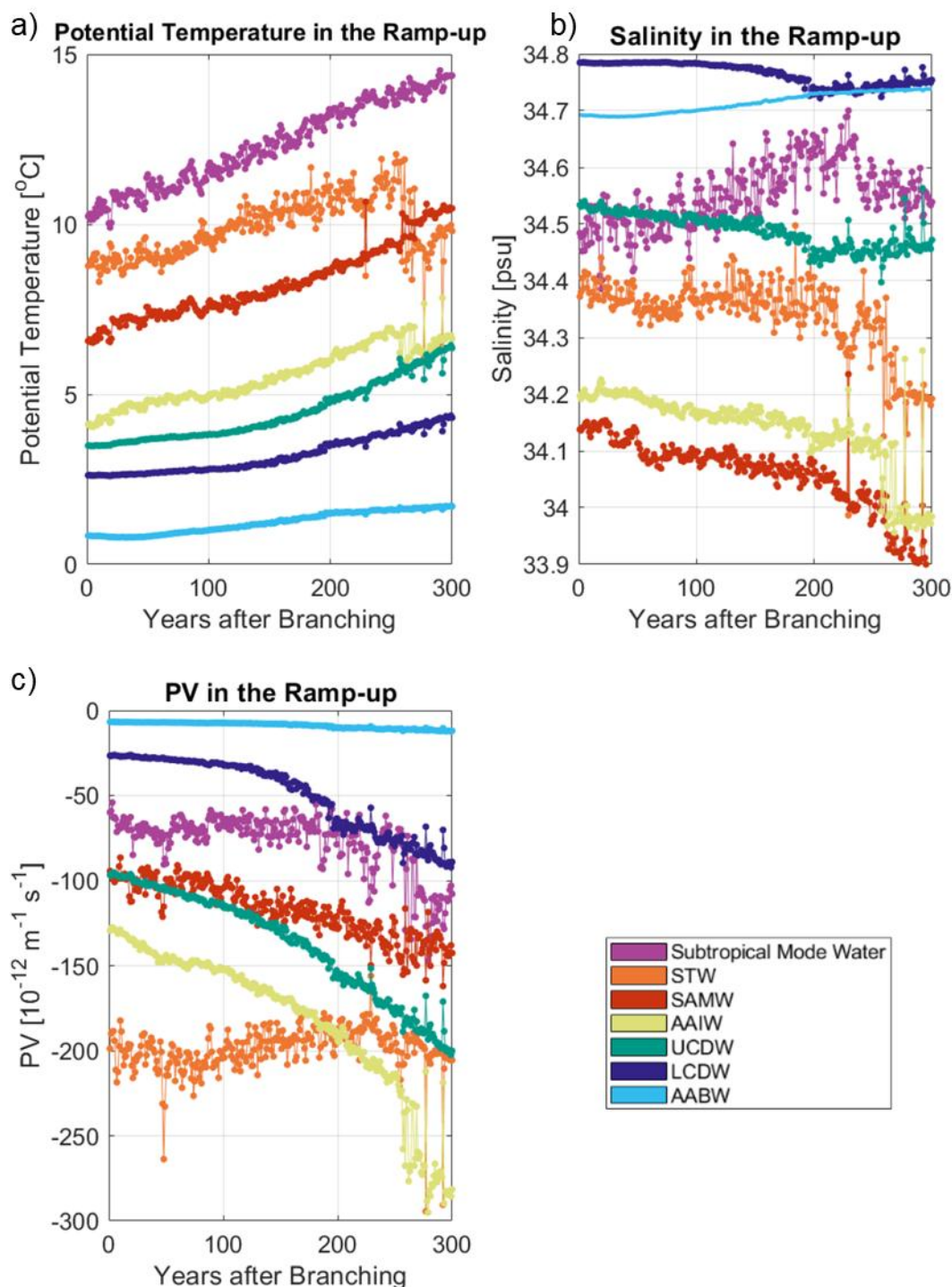


Figure 9: Same as Fig. 6 but for the evolution of potential temperature (top left), salinity (top right), and PV (bottom left) under the CO₂ ramp-up.



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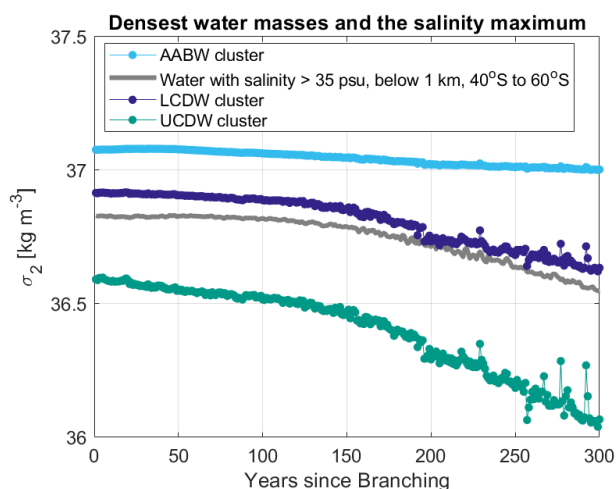


Figure 10: Same as Fig. 6 but comparing UCDW, LCDW, and AABW against the density of the deep salinity maximum.

We furthermore probe the persistence of temperature and density anomalies under reversing CO₂ forcing. We see
 405 that under a moderate warming of up to +2°C, the positive temperature and negative density anomalies of intermediate and
 mode water masses exhibit relatively easier reversibility, which can be contrasted against: 1) the less easily reversible
 temperature and density anomalies after a peak global warming of +4°C (Fig. 14) and 2) against the relative persistence of
 anomalies in the deep and bottom layers both after +2°C and +4°C global warming.

The clustering results for temperature and density are marked by less numerical noise compared to the results for
 410 salinity (compare Fig. 11 and 14). All watermasses in the region of interest show negative changes in density that persist on
 a centennial timescale after a +4°C global warming peak (Fig. 14, 15). All relatively persistent anomalies (except for AAIW
 temperature) exceed 2 standard deviations in the PI control variability (Fig. 15) after CO₂ is reduced following the +4°C
 global peak. In addition, CDW and AABW show persistent warming even after a +2°C global warming peak.

Another surprising result is that the thin Subtropical Thermocline Water layer shows noticeable difficult-to-reverse
 415 changes in temperature and density under a more modest warming (Fig. 14). However, this thermocline layer is not a
 coherent water mass, but is made up of spatially and temporally varying and disconnected volumes of water, and therefore, it
 is difficult to discuss their reversibility in a physically meaningful fashion.

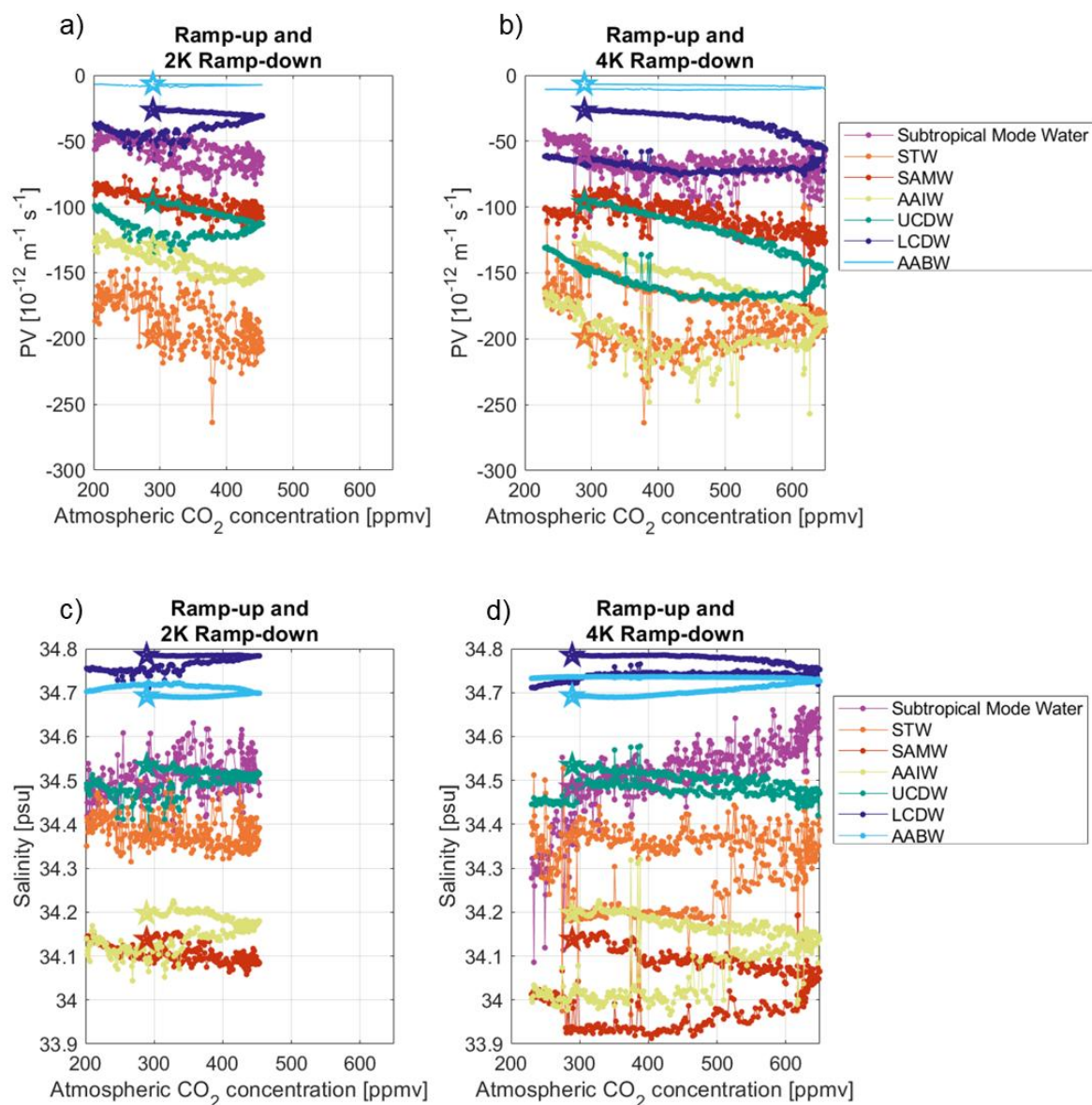


Figure 11: Transient hysteresis-like behaviour of PV [$\text{m}^{-1}\text{s}^{-1}$] (top) and salinity [psu] (bottom), during the sequence of CO₂ ramp-up, stabilization, and ramp-down reaching global warming levels of +2°C (top) and +4°C (bottom). Pointed star markers indicate the starting points.

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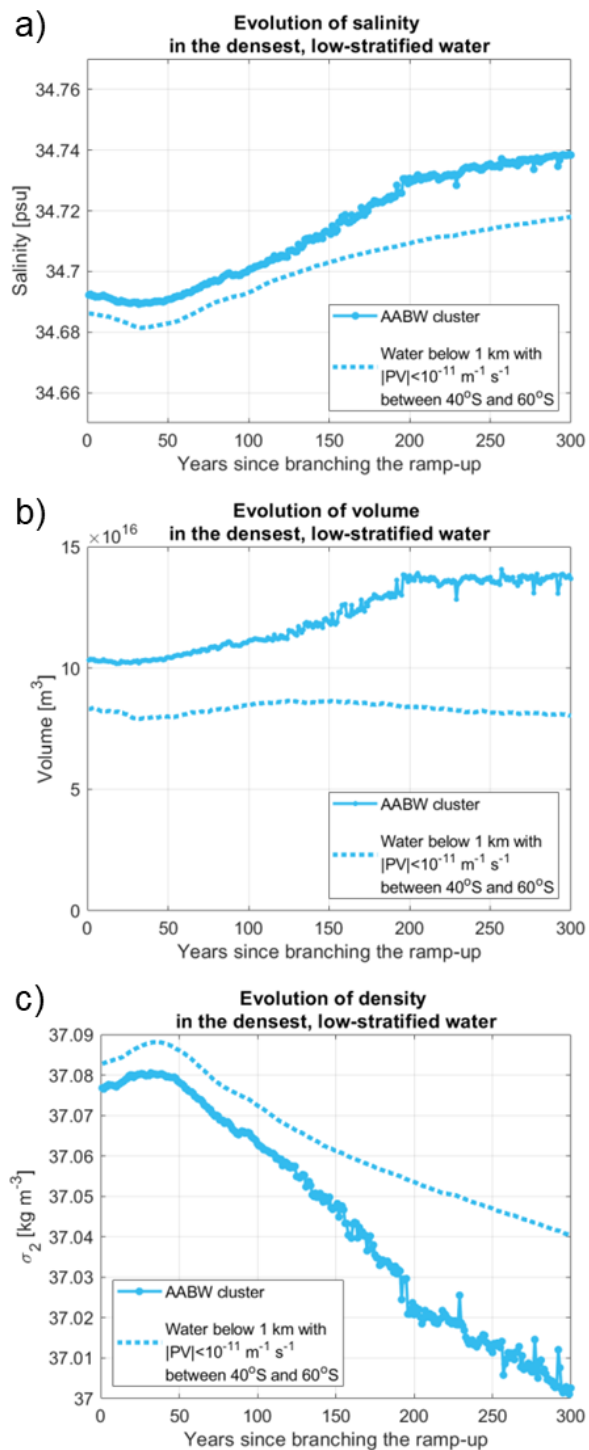
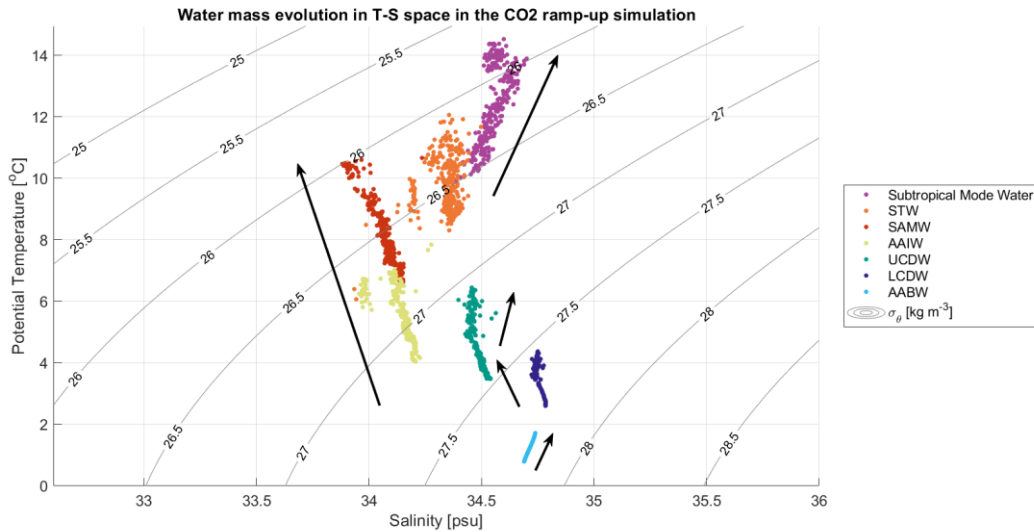


Figure 12: Evolution of salinity (top), water mass volume (middle), and potential density (bottom) in the AABW cluster and in the low-stratified water below 1 km with $|PV| < 10^{-11} \text{ m}^{-1} \text{ s}^{-1}$ in the domain of interest.



430 **Figure 13: Evolution of water masses in Temperature – Salinity space during the CO2 ramp-up simulation, as indicated with arrows. Superimposed are σ_θ potential density contours.**

3.2 Water mass volume and heat content

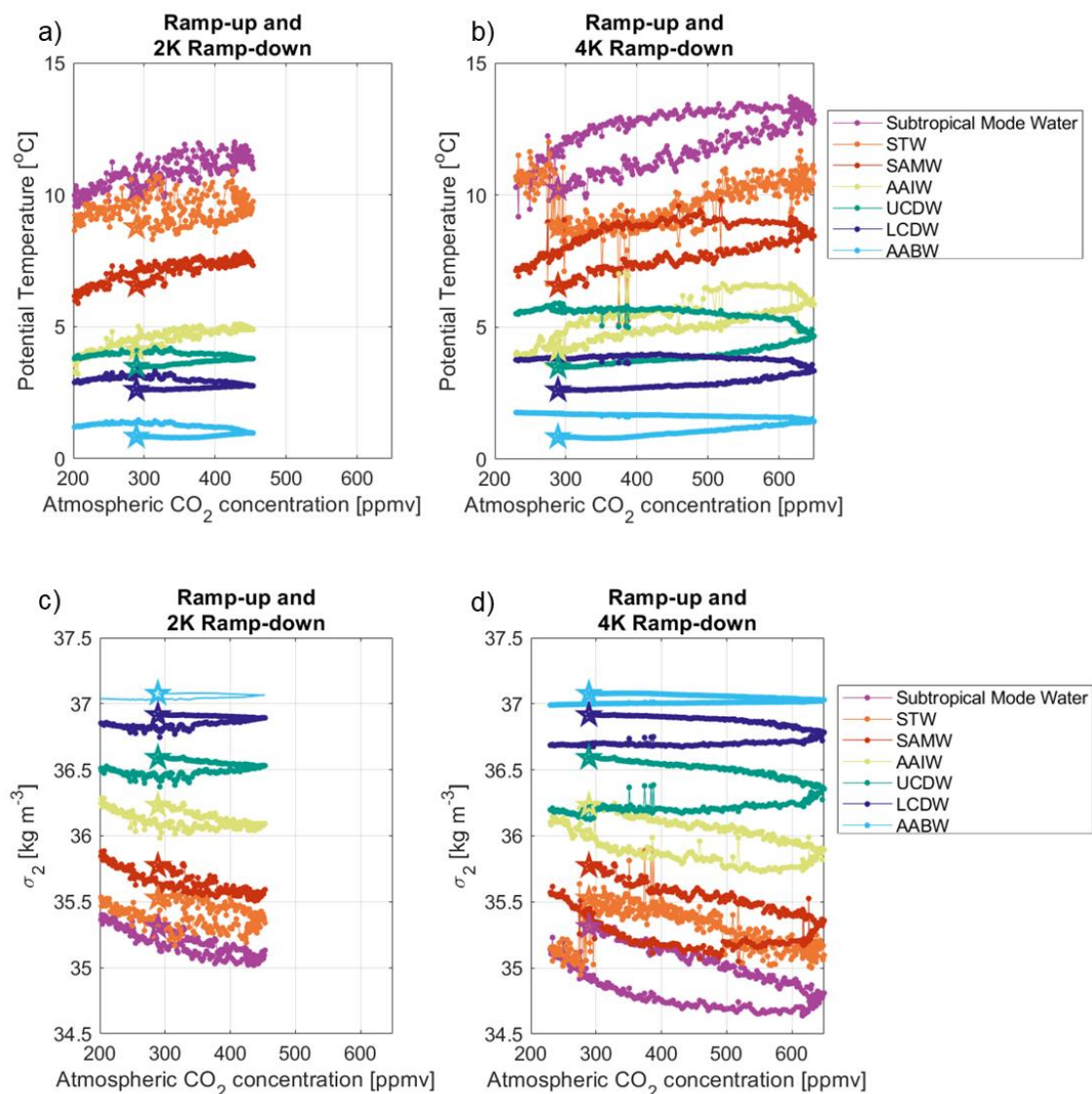
A specific advantage of our algorithm is the ability not just to label water masses, but also to identify well-defined water mass volumes (Fig. 16). It is particularly notable that under CO2-induced warming, the volume of SAMW remains approximately the same, while the volume of April AAIW decreases (Fig. 16). Another important result concerns the volumes of Bottom Water and Circumpolar Deep Water varieties. Under CO2 ramp-up, the local volume of accumulated AABW increases despite the cessation in the import of new (young) AABW from the south. The AABW volume anomaly is sustained on centennial timescales even under negative CO2 emissions that bring down the atmospheric greenhouse gas concentrations to preindustrial levels. When we analyse the least stratified water below a depth of 1 km, we do see a small, possibly transient, increase in its volume (Fig. 12). Our AABW cluster captures this stratification minimum. However, the AABW cluster also spans neighbouring relatively low-stratified layers located between the $|PV|$ minimum ($|PV| < 10^{-11} \text{ m}^{-1} \text{ s}^{-1}$) near the bottom and the salinity maximum, which falls into the adjacent LCDW cluster. Therefore, we do not expect the volume of the AABW cluster to exactly match the volume of deep/bottom water with $|PV| < 10^{-11} \text{ m}^{-1} \text{ s}^{-1}$.

In contrast to the AABW cluster, LCDW volume decreases under a CO2 ramp-up (Fig. 16). The main source of LCDW is North Atlantic Deep Water, flowing southward along the lower branch of the upper cell of the Atlantic Meridional Overturning Circulation (AMOC), which weakens and shoals under increased CO2 forcing (e.g., Kostov et al., 2014). The weakening of the AMOC causes a reduction in the southward flow supplying high salinity, low-stratified (but more stratified than AABW) precursors to LCDW (Fig. 7).

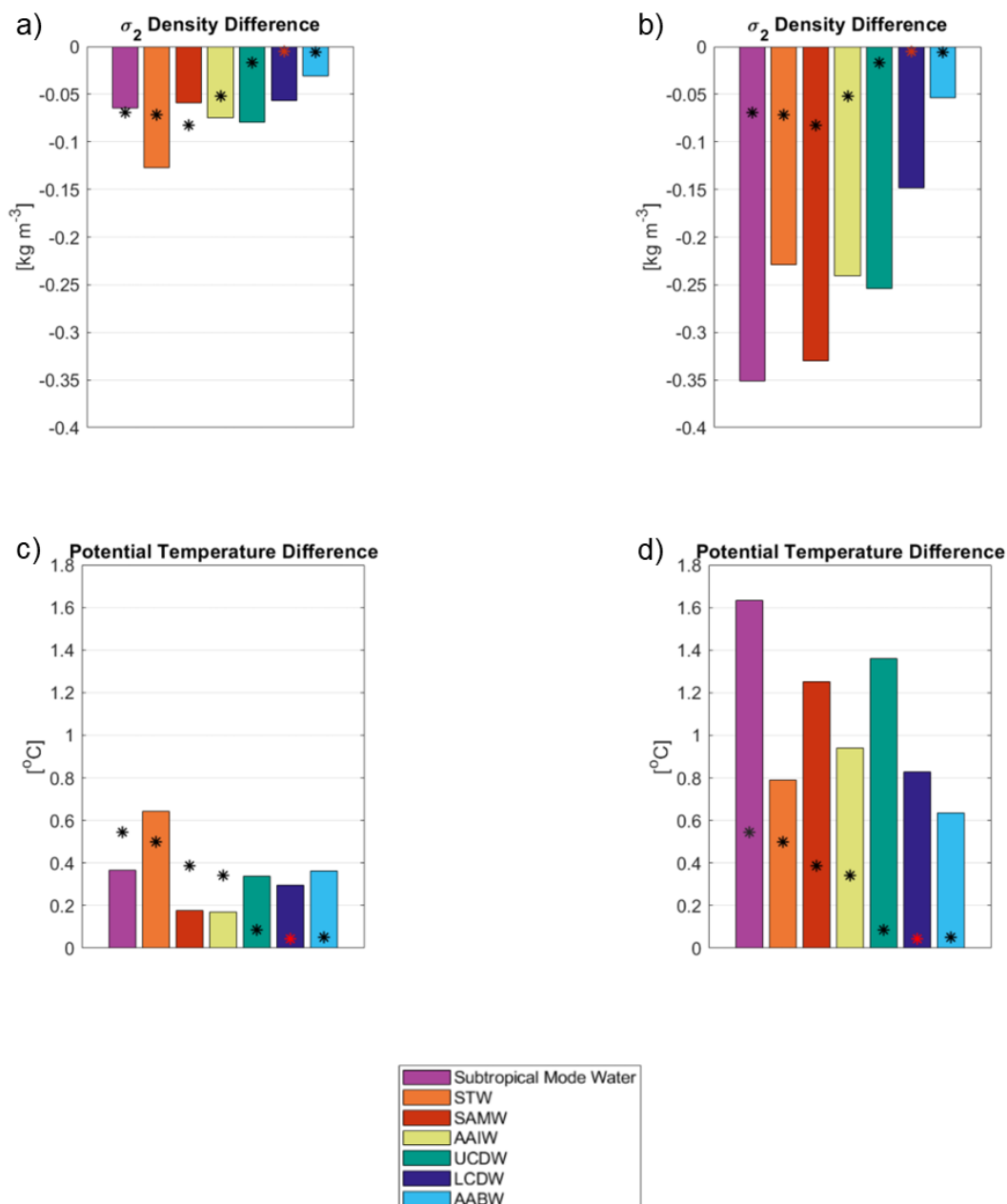


450 It is noticeable that the local increase in accumulated AABW is achieved at the expense of the LCDW volume (Fig. 16). As discussed, the AABW and LCDW water masses are less and less efficiently replenished with new precursors as the CO₂ ramp-up simulation advances. The mixing between the old reservoirs of AABW and LCDW, as well as their precursors, has an impact on the water mass volumes. In our domain, AABW has a larger volume than LCDW, and as the two water masses and their respective precursors mix, AABW properties dominate, thereby giving rise in the expansion of AABW at the expense of the adjacent LCDW (Fig. 16).

455



460 **Figure 14: Transient hysteresis-like behaviour of potential temperature [°C] (left) and potential density σ_2 [kg m⁻³] (right) during the sequence of CO₂ ramp-up, stabilization, and ramp-down reaching global warming levels of +2°C (top) and +4°C (bottom). Pointed star markers indicate the starting points. Note that STW is not a spatially coherent water mass but represents pockets of highly-stratified water adjacent to the low-stratified SAMW.**



465 **Figure 15: Residual anomaly in potential temperature [$^{\circ}\text{C}$] (top) and potential density σ_2 [kg m^{-3}] (bottom) after a sequence of CO₂ ramp-up, stabilization, and ramp-down to the initial preindustrial levels. The anomalies are computed relative to the first year of the ramp-up. In the left column, we reach peak global warming levels of +2 $^{\circ}\text{C}$ (top) and in the right, +4 $^{\circ}\text{C}$ before stabilisation and ramp-down. Asterisk markers indicate 2 standard deviations in the PI control April climatological interannual variability in the properties of the respective water masses.**

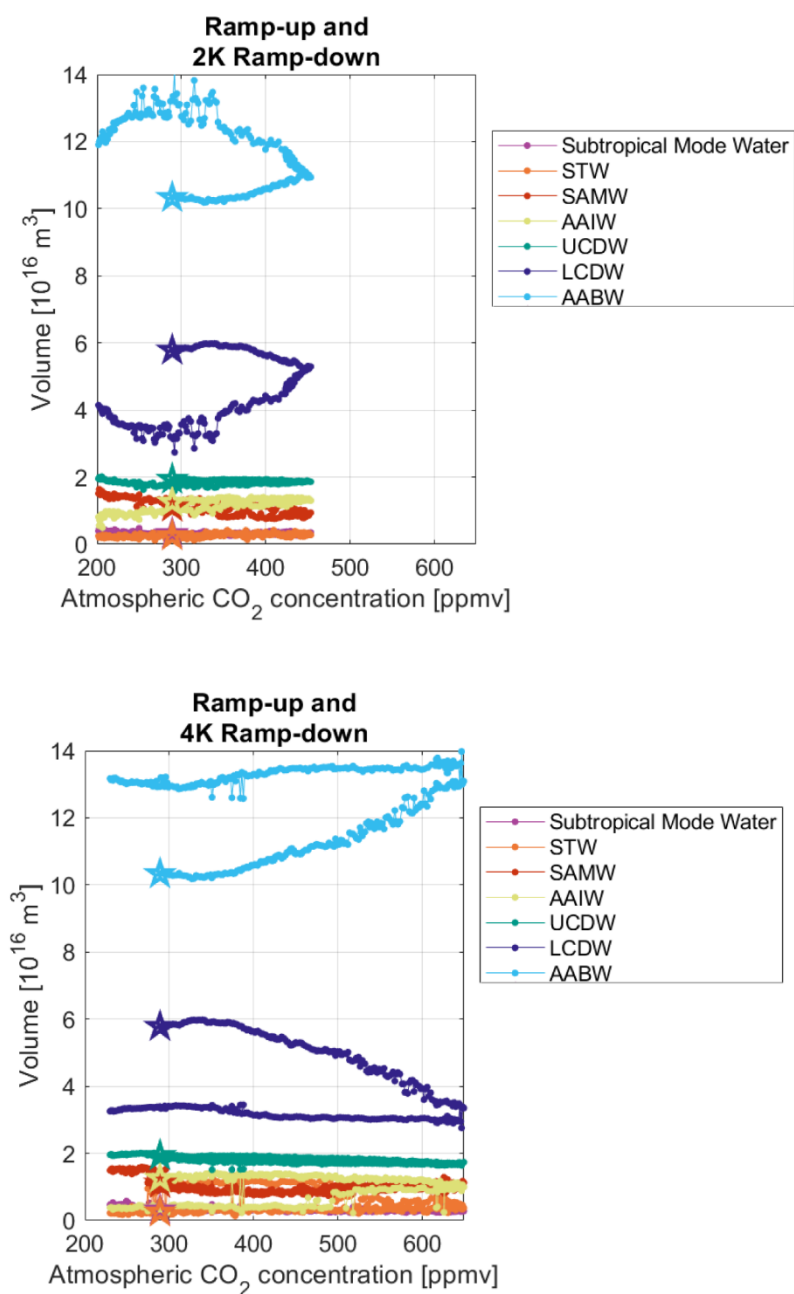
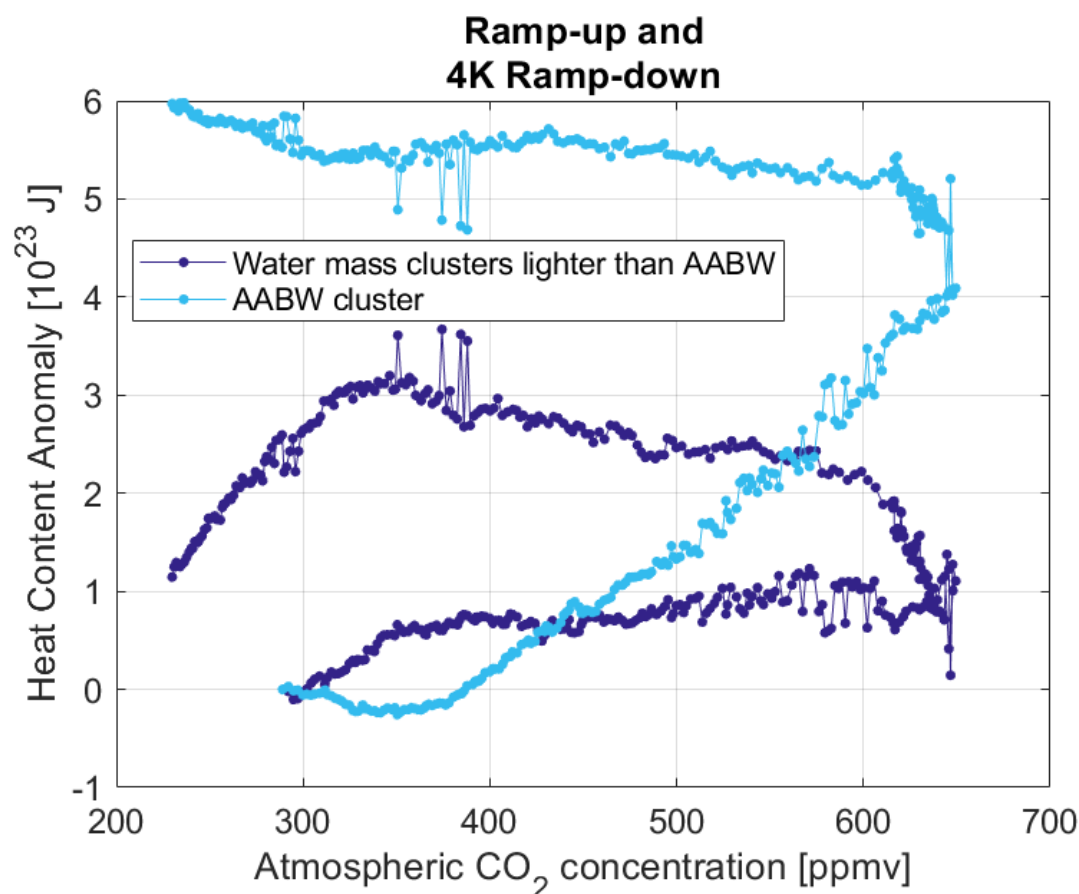


Figure 16: Transient hysteresis-like behaviour of water mass volume [10^{16} m^3] during the sequence of CO_2 ramp-up, stabilization, and ramp-down after global warming levels of $+2^\circ\text{C}$ (top) and $+4^\circ\text{C}$ (bottom).

Using the temperature and volume anomalies (Fig. 14 and 16), we then compute the heat content anomalies for each layer, as it evolves in time (Fig. 17). However, if we consider all layers lighter than AABW as a whole, we see that their



ocean heat content anomaly remains positive and does not decrease in magnitude, as the CO₂ concentration is lowered all the way until it is restored to PI levels (Fig. 17). In AABW, there is also a large positive heat content anomaly that does not decrease even when CO₂ concentrations are brought down below preindustrial levels (Fig. 17).



480 **Figure 17: Heat content anomaly in different water masses under a CO₂ ramp-up to a +4°C warming, followed by stabilisation and a CO₂ ramp-down below the initial PI concentration.**

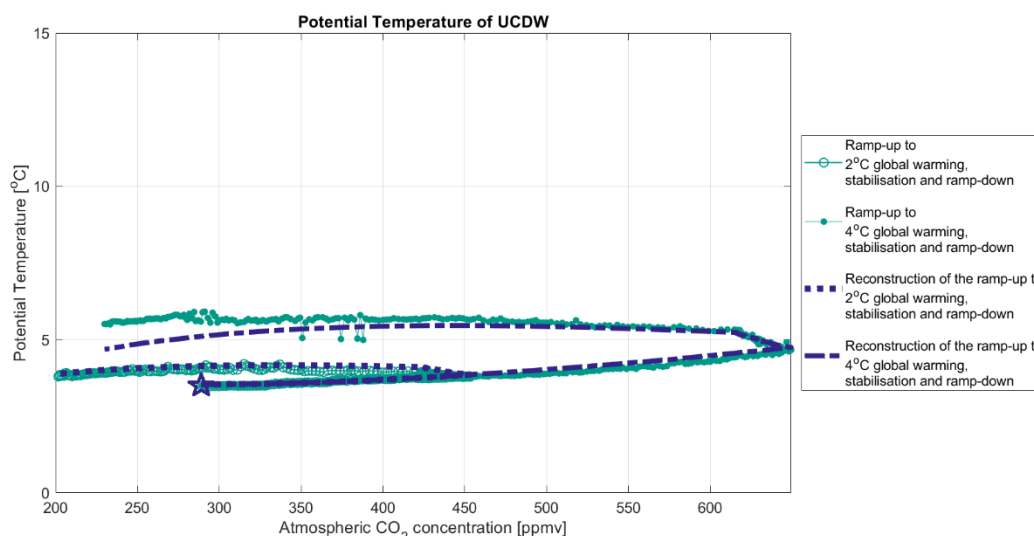
485 **3.2 Centennial persistence and potential long-term reversibility**

Our results indicate that properties of individual water masses exhibit persistence on centennial timescales in response to an increase followed by a decrease in CO₂. However, this does not necessarily imply absolute irreversibility of these anomalies on longer timescales or the existence of multiple equilibria for these ranges of CO₂ concentrations.



For example, a multi-centennial exponential timescale of response to CO₂ forcing (see Appendix E) is
 490 qualitatively consistent with the evolution of potential temperature in the UCDW cluster, a water mass whose property
 anomalies persist after a +2°C global warming peak. Assuming an idealised asymptotic decay of the anomaly on a 300-year
 characteristic timescale (Fig. E1 in Appendix E), allows us to recover hysteresis-like loops (Fig. 18) very similar to the
 results in Fig. 14 a and b. Mismatches between the example idealised reconstruction and the temperature evolution (Fig. 18)
 may be due to the presence of an adjustment timescale longer than 300 years, multiple timescales of response, or a non-
 495 monotonic response rather than a simple exponential decay. In addition, the temperature response may exhibit non-linear
 characteristics. However, this does not automatically mean that we have reached multiple possible equilibria under the same
 atmospheric CO₂ concentration.

Our results are therefore consistent with long-term inertia in the subantarctic response and do not necessarily tell us
 whether a true underlying hysteresis in the mathematical sense of the word is present. Conversely, our findings do not rule
 500 out the existence of multiple equilibria, and our results are scenario-specific. For example, a more abrupt increase in
 atmospheric CO₂ concentrations may irreversibly push the system to a different steady state.



505 **Figure 18: Idealised reconstructions of the UCDW temperature responses (Fig. 14 a,b) to CO₂ ramp-up to 2°C and 4°C followed by ramp-downs. The idealised reconstructions assume a linear response with a 300-year exponential timescale of decay (see Appendix E). A star indicates the beginning of the CO₂ ramp-up and ramp-down cycles.**

4 Discussion and conclusions

Our results support the findings of Sallée et al. (2013) that the most consistent response across all water masses under a
 simulated increase in CO₂ forcing is a warming and lightening throughout the entire water column. The largest and most
 510 persistently large temperature and density anomalies under CO₂ ramp-up are found in the subtropical waters, in Circumpolar



Deep Waters whose primary source is North Atlantic Deep Water, as well as in Bottom Waters. The subtropical water masses quickly reach large temperature anomalies because of their smaller volume. In contrast, the deeper water masses that are ventilated further poleward have larger reservoirs, whose volume effectively buffers and delays the warming response. On the other hand, the same buffering effect means that the deep ocean layers, especially the ones mixed with remotely-sourced North Atlantic Deep Water, have the slowest recovery rate for temperature and density when we reverse from CO₂ ramp-up to stabilisation and ramp-down. Our model results do not agree with those of Sallée et al. (2013) in the response of SAMW and AAIW to CO₂ ramp-up: we find that despite their efficient local exposure to the atmosphere in the domain of interest, these intermediate and subpolar mode water masses warm at the same rate as subtropical layers and UCDW.

After a +2°C global warming peak, the intermediate and mode water mass temperature and density anomalies disappear as CO₂ is lowered back to PI values, suggesting that such changes remain reversible under moderate CO₂ increase scenarios. They return to values comparable to the PI simulation well within the expected margin of natural variability. However, if CO₂ is lowered after a +4°C global warming peak, even the intermediate and mode water mass temperature and density anomalies persist and at the time when CO₂ concentrations once again reach ~290 ppm, the persistent anomalies exceed several times the magnitude of natural variability found in the PI control simulation. This demonstrates a nonlinear shift in the water mass responses that depends on the warming levels and shows potential for some degree of persistence on centennial timescales. However, the temperature anomalies of Subtropical LCDW, and AABW, which exhibit centennial irreversibility in warming even after a 2°C global warming peak.

All subantarctic water masses become more strongly stratified under increased greenhouse gas forcing, and for UCDW, LCDW, and AABW this enhanced stratification does not reverse when CO₂ concentrations are lowered. AAIW exhibits a similar persistent stratification enhancement if peak global warming levels of 4°C are reached.

In addition, we find centennially persistent responses in ocean salinity. Unlike the reversible salinification of Subtropical Mode Water, our AABW cluster exhibits persistent salinification, which is separately confirmed by directly analysing the low-stratified water below a depth of 1 km. The long-term salinification of AABW in a warming world agrees with the results of Gunn et al. (2026). In contrast to AABW, AAIW, UCDW, and LCDW show persistent freshening. SAMW also shows centennial persistence in freshening but only under the high warming scenarios (exceeding 0.2 psu of freshening for SAMW, Fig. 11).

We also identify an important feature in Indo-Pacific SAMW both in the PI climatology and the CO₂ ramp-up and ramp-down. In the PI climatology, similar to present day conditions, only the Atlantic Sector of the Southern Ocean exhibits sharp gradients between Subtropical Mode Water and SAMW (Fernández Castro et al., 2025). The model's climatology is thus in line with studies demonstrating direct connectivity between Subtropical Mode Water and SAMW in the Indo-Pacific sector, whereby subtropical sources contribute substantially to the local varieties of SAMW (Fernández Castro et al., 2025) in contrast to the separation between Subtropical Mode Water and SAMW in the Atlantic Sector. However, our model predicts that under very high emission scenarios, SAMW switches to a new regime marked by more spatially intermittent formation sites separated by regions of high stratification that prevent the convective formation of mode water.



545 Knowing both the temperature and volume evolution of water masses (a key advantage of our algorithm to other machine learning classification methods) allows us to compute the changing water mass heat content anomalies. There is substantial compensatory variability between adjacent layers, especially during the CO₂ ramp-down, primarily because of volume rather than temperature anomalies. However, heat content anomalies exhibit noticeable persistence across layers. The positive heat content anomaly in AABW layers continues to grow even as CO₂ is ramped down all the way to preindustrial atmospheric conditions.

550 Our findings have relevance not only for future changes in ocean heat, but also for carbon storage under increased anthropogenic greenhouse gas forcing: SAMW, AAIW, and AABW contribute to the uptake and storage of anthropogenic carbon and heat at depth, while CDW is an important source of outgassed carbon and upward heat transport that can enhance the Antarctic iceshelf rates of melting.

555 However, the reliance on a single model in our study is a limitation. This UKESM coupled configuration appears to have a warm bias in part of the region and depth range we consider. In contrast to the model intercomparison of Sallée et al. (2013), our largest warm bias is found in UCDW rather than in the locally sourced water masses. At the same time, we demonstrate that our k-means clustering approach is not affected by features specific to a given model configuration no matter whether we consider the preindustrial climatology, warming scenarios, or cooling scenarios.

560 The fact that our cluster boundaries are not material surfaces limits our ability to apply the classical surface water mass transformation framework (Speer and Tziperman, 1992; Abernathey et al, 2016; Desbruyères et al., 2019; Kostov et al., 2023; Fu et al., 2024) or analyse the water mass budget using the established approach by Walin (1982). The aforementioned studies rely on density bounds and density surface approximations to material surfaces.

565 Nevertheless, the advantage of our algorithm is that despite its limitations, we can track “functional” water masses as they themselves shift their position in density space under the effects of greenhouse gas forcing. We achieve this by building upon the approach by Sallée et al. (2013) but in a novel machine learning framework that leaves little room for subjective and arbitrary choices in delimiting water masses in a changing climate. Our results about the warming, lightening, and increased stratification imply a reduction in the future ability of a warmer subantarctic ocean to store additional anthropogenic heat and carbon at depth. Of particular importance is the persistence of these thermodynamic changes in the deep and abyssal ocean layers on centennial timescales even after a reduction in atmospheric CO₂ concentrations. Finally, even though our analysis cannot establish or rule out absolute irreversibility and multiple equilibria in the system, the potential for persistence in subantarctic water mass anomalies on centennial timescales is relevant to the analysis of future greenhouse gas emission scenarios and their impact on climate.



575 Appendix A. Gap value criteria for the k-means clustering algorithm

The gap value criterion is a measure of the clustering skill and can capture a potential trade-off between the ability to cluster data points and the number of clusters k . We use the gap value criterion defined with the standard expression:

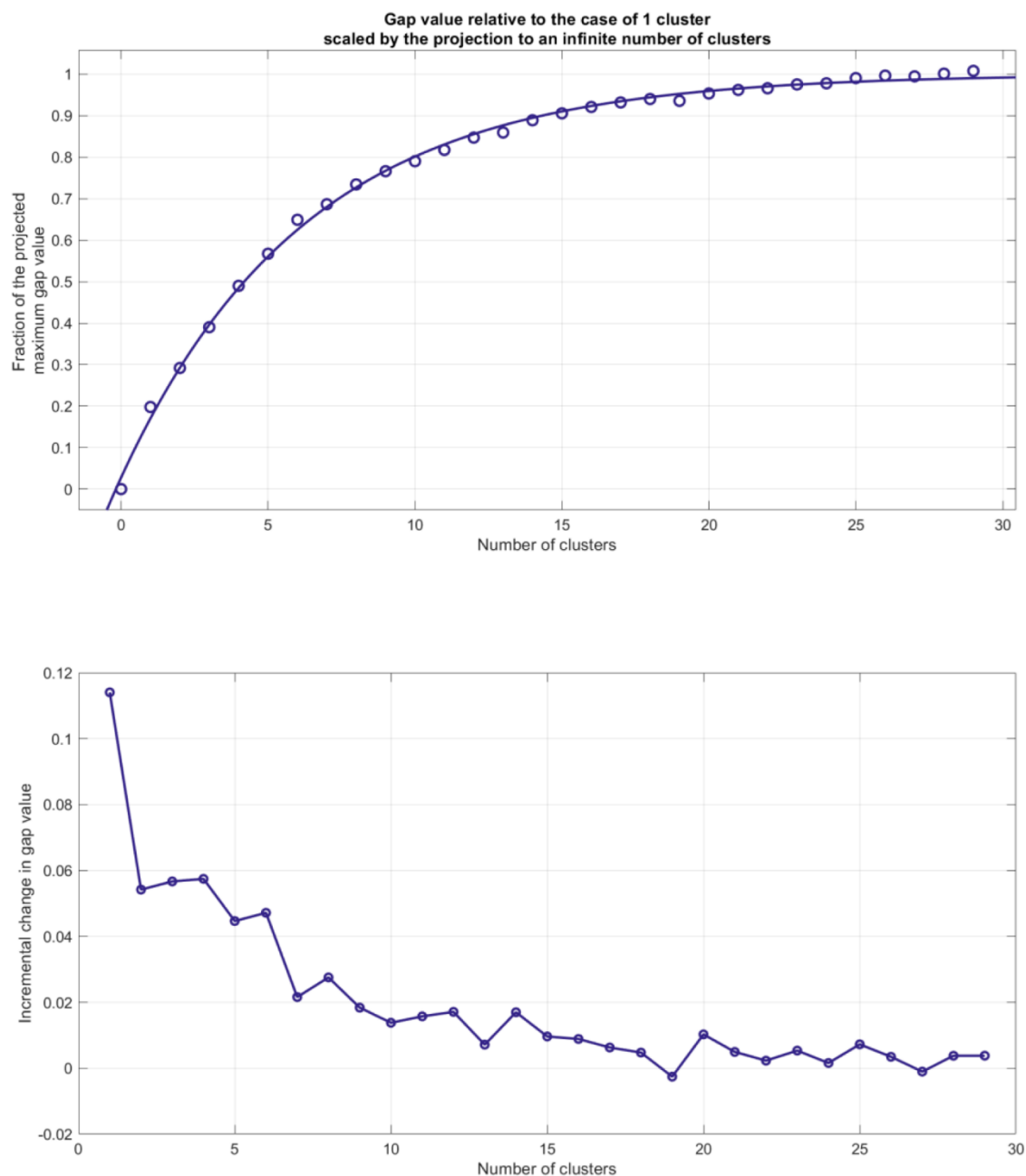
$$Gap_n(k) = E_n^*\{\log(W_k)\} - \log(W_k), \quad (A1)$$

580 where n represents the sample size, k represents the number of clusters. The sum of the dispersion within each of the k clusters W_k is defined as

$$W_k = \sum_{r=1}^k \frac{1}{2n_r} D_r, \quad (A2)$$

where n_r is the number of data points in each cluster r , and D_r is the sum of all distances between each pair of points in that cluster. Monte Carlo sampling from a uniform distribution gives the expected value $E_n^*\{\log(W_k)\}$, while $\log(W_k)$ is computed from the actual sample data.

585 We consider the gap value for $k = 1..30$ clusters (Fig. A1), where we find that the value is monotonically increasing. We successfully fit an asymptoting exponential term to extrapolate the gap value to a hypothetical case of hundreds of clusters. We then rescale the results for the gap value by the extrapolated magnitude and compare results relative to the trivial case $k = 1$ (Fig. A1). In addition, we calculate the incremental increase in gap value with each increase in the cluster number k (Fig. A1).



590

Figure A1: Top: Gap value when varying the number of clusters k in the algorithm applied to the PI April climatology. A shifted gap value is shown relative to the case of 1 cluster and is rescaled by the projection of the exponential fit to infinity; Bottom: Incremental improvement of the gap value with each cluster number increment.



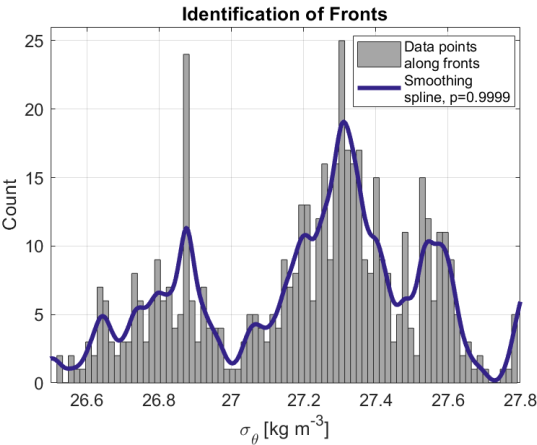
595 **Appendix B. Initial cluster centroid properties**

Table B1: Initial starting points for the cluster centroid properties

Cluster Number	Label	Potential Temperature [°C]	Salinity [psu]	PV [$10^{-12} \text{ m}^{-1} \text{ s}^{-1}$]
1	Subtropical Mode Water	13.80	34.97	-50
2	STW	10.00	34.50	-200
3	SAMW	8.02	34.49	-75
4	AAIW	4.14	34.28	-100
5	UCDW	3.25	34.76	-100
6	LCDW	1.37	34.80	-75
7	AABW	-0.22	34.68	-0.1

Appendix C. Identification of fronts

We consider the ocean fronts in our domain of interest, as represented in the model simulations. We examine the April σ_θ potential density in Year 201 of the PI Control, when we start our analysis, and we focus on a subsurface model layer at a depth of 370m. We apply the Gonzalez (2026) ocean front detection algorithm, selecting the Canny (1986) method for identifying fronts.



605 **Figure C1: Histogram of the data points along the detected Canny (1986)-type fronts in σ_θ potential density at 370m. The data points are shown in σ_θ space and grouped into 80 bins. Superimposed is a smoothing spline with a roughness parameter $p=0.9999$.**

We then examine all points through which the automatically detected fronts pass. There are discontinuities in these Canny (1986)-type fronts, and some of them intersect density levels. We consider the distribution of the points along the



610 Canny-type fronts in σ_θ space and fit a smoothing spline with a roughness parameter $p=0.9999$ (Fig. C1). Finally, we identify peaks in the smoothed distribution fit as projections of the Canny-type fronts onto potential density. This allows us to connect the initially discontinuous fronts in a circumpolar sense.

615 We identify three peaks in the fit in Fig. C1 as known fronts: the Subtropical Front (STF) at $\sigma_\theta = 26.64 \text{ kg m}^{-3}$, the Subantarctic Front (SAF) at $\sigma_\theta = 26.88 \text{ kg m}^{-3}$, and the Polar Front (PF) $\sigma_\theta = 27.31 \text{ kg m}^{-3}$ and compare them against our clustering results (Fig. C2a). We see that the SAF and PF match very well our expected boundaries between SAMW and AAIW and between AAIW and UCDW, respectively (Fig. C2a). The estimated STF shows good agreement with the northern boundary of the SAMW cluster in the Atlantic and part of the Indian Sectors. However, our estimated STF is clearly biased heavily towards matching the ocean front in the Atlantic and Indian Oceans and does not skilfully track the water mass boundary in the Pacific Sector (Fig. C2). We therefore show the $\sigma_\theta = 26.64 \text{ kg m}^{-3}$ contour as the STF only in the Atlantic and Indian Sectors, while it is clear that the STF is located further northward in the Pacific.

620 We also compare our estimates of the model fronts against the observationally-derived Park et al. (2019) Southern Ocean fronts, namely the SAF and the PF (Fig. C2b). We see that there is overall good agreement between our fronts calculated for the model's PI experiment and present day observations. However, in April of Year 201 in the PI simulation, we find a greater northward extent of AAIW compared to modern day observations (Compare Fig. C2 a and b).

625

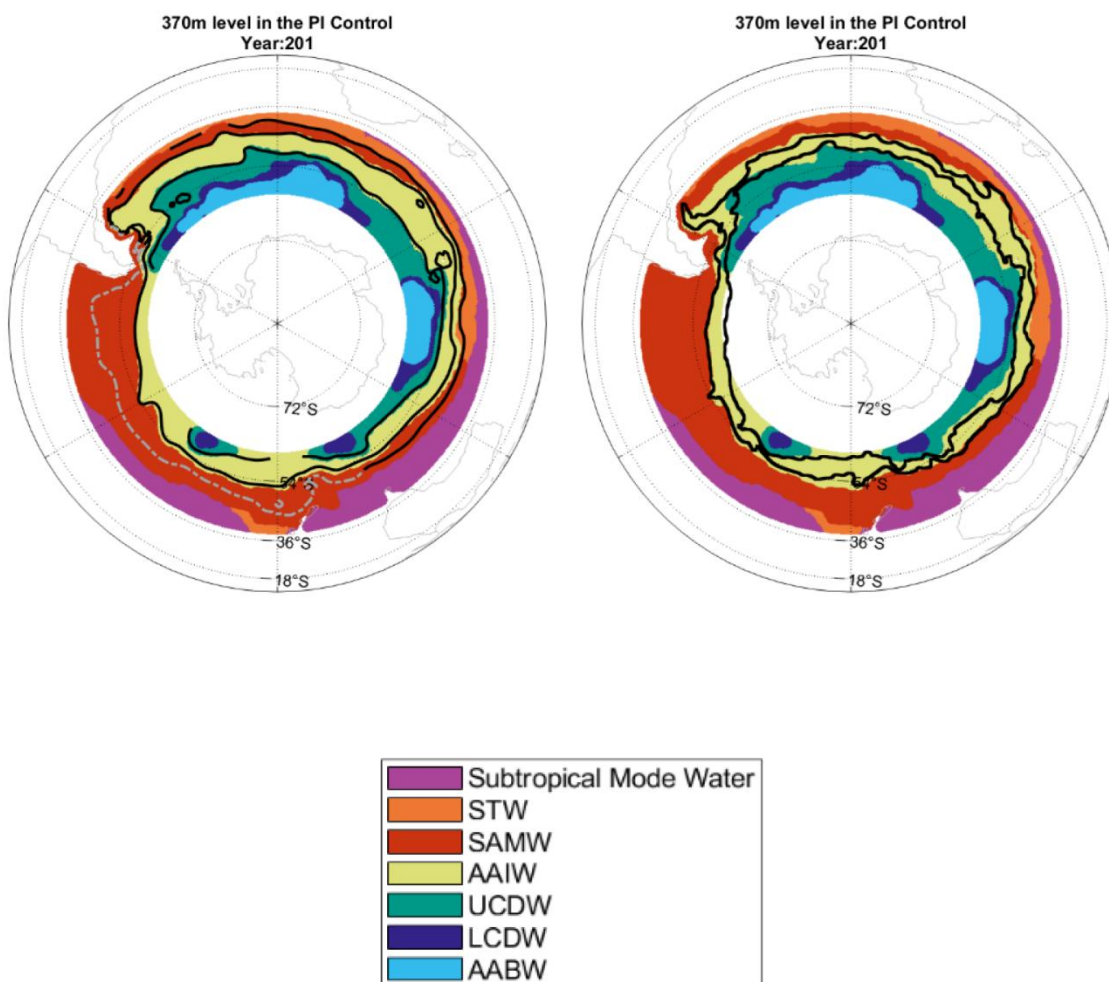


Figure C2: Result of the clustering algorithm at a depth of 370 m in Year 201 of the PI simulation with a) superimposed fronts as estimated for this time period in the model simulation (replicated from Fig. 4 in the main text); b) observationally-based location of major fronts from Park et al. (2019).



Appendix D. Qualitative regime changes in SAMW under strong warming scenarios

SAMW regime shifts do not appear in the model's PI control simulation, or under moderate global warming up to +2°C. Here we highlight the abrupt change in the nature of SAMW that emerges under global warming greater than +4°C, including cases of continued positive CO₂ emissions, as well as CO₂ ramp-down after a +4°C global warming peak.

Under as CO₂ ramp-down after a +4°C global warming peak, the subantarctic Southern Ocean continues to warm. As SAMW becomes warmer and more stratified, there is an abrupt emergence of a new SAMW state, where, the continuous circum-Antarctic band of SAMW is replaced by a set of spatially disconnected volumes of water. They are surrounded by even more highly stratified STW, where the latter even reaches the denser AAIW layer that lies to the south of SAMW (Fig. D1a). Such a regime shift in SAMW also appears when the CO₂ ramp-up experiment is extended to global warming levels greater than +4°C (Fig. D1b), which demonstrates that the regime shift is a forced response to warming.

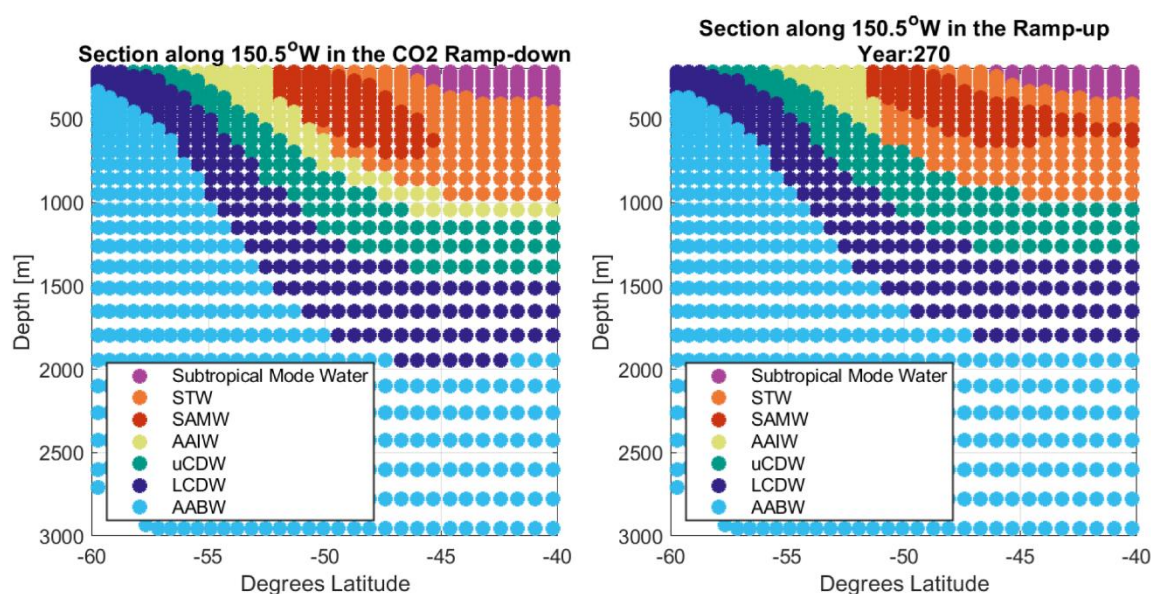


Figure D1: Emergence of a new SAMW regime. a) A new SAMW fingerprint in Year 51 of the CO₂ ramp-down; c) A similar new SAMW fingerprint emerging in an extension of the ramp-up simulation beyond a global warming level of +4°C.



650 Appendix E. Multi-centennial exponential response timescales

We consider a hypothetical idealised response function for the evolution of UCDW potential temperature under an impulse perturbation in the atmospheric CO₂ concentration. We assume that the response function $F(\tau)$ is marked by a simple exponential decay over time lag τ with a single timescale of 300 years (Fig. E1) and therefore proportional to $F_0(\tau)$ defined as:

$$655 \quad F_0(\tau) = e^{-\tau/300} \quad (E1)$$

We then convolve the exponential function from Eq. (E1) with the timeseries of atmospheric CO₂ concentration [CO₂] anomaly in a CO₂ ramp-up simulation (Fig. E1) to obtain a response:

$$\text{Convolution} = \int_0^t \int_0^{300} F_0(\tau) [\text{CO}_2(t - \tau)] d\tau dt = \int_0^t \int_0^{300} e^{-\tau/300} [\text{CO}_2(t - \tau)] d\tau dt \quad (E2)$$

Finally, we linearly scale the convolution in Eq. (E2) by a factor of $4.21 \times 10^{-5} \text{ }^\circ\text{C ppmv}^{-1} \text{ year}^{-1}$ to best match the evolution of UCDW in the ramp-up simulation (Fig. E2). We therefore obtain an idealised linear response function,

$$F(\tau) = 4.21 \cdot 10^{-5} F_0(\tau) = 4.21 \cdot 10^{-5} e^{-\tau/300} \quad (E3)$$

for the evolution of UCDW temperature under atmospheric CO₂ perturbations. By analogy to Eq. (E2), we can then convolve $F(\tau)$ from (E3) with the timeseries of atmospheric CO₂ as the latter is ramped down after a 2°C and a 4°C global warming peak (Fig. E2). Considering these responses as a function of CO₂ concentration rather than time allows us to produce the idealised responses of Fig. 18 in the main text.

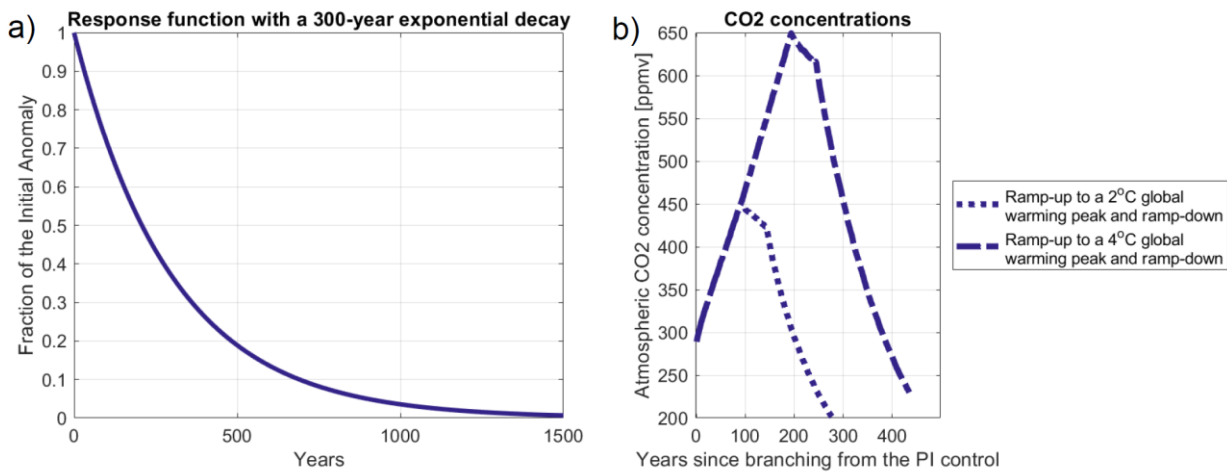


Figure E1: a. Idealised exponential decay with a timescale of 300 years. b. Evolution of the CO₂ atmospheric concentrations under different scenarios.

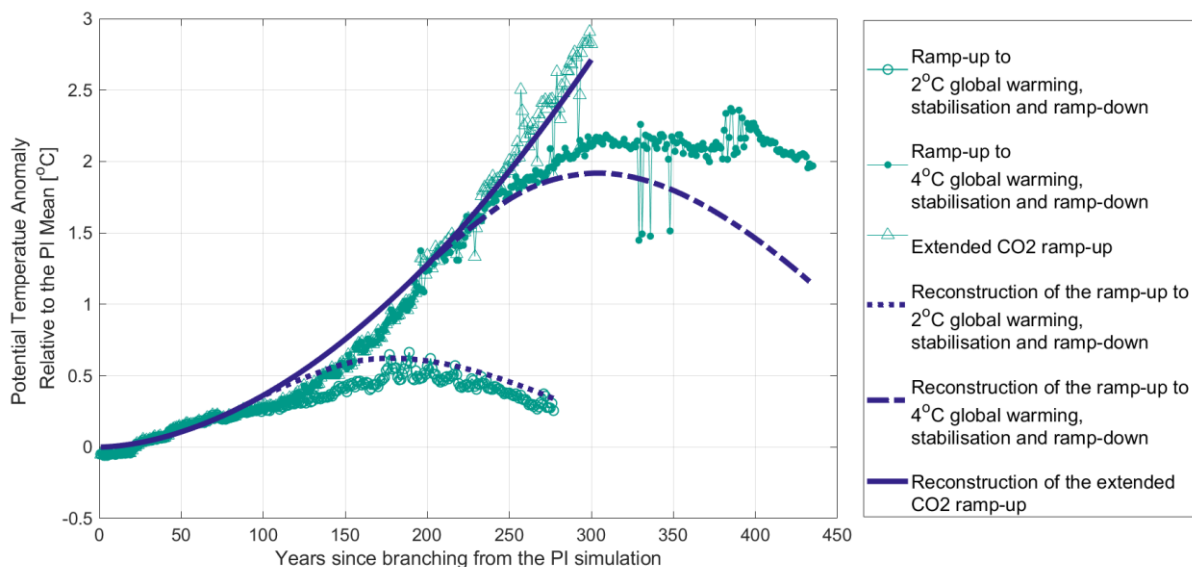


Figure E2: Convolution of the scaled response function with the CO₂ concentration from the ramp-up simulation, as well as two different ramp-down scenarios after a 2°C and 4°C global warming peak, respectively.

Code and data availability

Essential output from the UKESM TIPMIP ensemble is CMORised and publicly available at <https://gws-access.jasmin.ac.uk/public/ukesm/TerraFIRMA>. The UKESM TIPMIP archive is stored at the UK Met Office and are accessible on the JASMIN research platform (www.jasmin.ac.uk) maintained by the Centre for Environmental Data Analysis (CEDA). The Gonzalez (2026) algorithm for front identification is available at <https://doi.org/10.5281/zenodo.20764811>. Code will further be made available upon the acceptance of this publication.

Author contributions

Conception: YK, PRH; Development of clustering algorithm: YK; Provided UKESM TIPMIP simulation output: RSS, JJ
 Analysed output: YK Provided manuscript content: YK, PRH, AJSM, RSS, JJ, AJP; Commented on manuscript content:
 YK, PRH, AJSM, RSS, JJ, AJP Contributed to obtaining funding: PRH, AJSM, RSS, AJP.

Competing interests

The authors declare no competing interests.



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695 Acknowledgements

The authors express gratitude for their access to the JASMIN and UK Met Office data facilities.

Financial support

This research was supported by Ocean Cryosphere Exchanges in ANtarctica: Impacts on Climate and the Earth system, OCEAN ICE, which is funded by the European Union, Horizon Europe Funding Programme for research and innovation
700 under grant agreement Nr. 101060452, <https://doi.org/10.3030/101060452>. OCEAN ICE contribution number 62. This work was funded by UK Research and Innovation (UKRI) under the UK government's Horizon Europe funding Guarantee grants 10048443, 10039016, and 10126975. The computer simulations and research in this study were supported by the UK Natural Environment Research Council through the TerraFIRMA: Future Impacts, Risks and Mitigation Actions in a changing Earth System project, Grant reference NE/W004895/1 and The UK Earth System Modelling Project, Grant 435 reference
705 NE/N017951/1. The authors acknowledge project TipESM “Exploring Tipping Points and Their Impacts Using Earth System Models”. TipESM is funded by the European Union, Grant Agreement number: 101137673. DOI: 10.3030/101137673.

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