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Article

Errors in Estimated Temporal Tracer Trends Due to Changes in the Historical Observation Network: A Case Study of Oxygen Trends in the Southern Ocean

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Abstract: Several models predict large and potentially abrupt ocean circulation changes due to anthropogenic greenhouse-gas emissions. These circulation changes drive-in the models-considerable oceanic oxygen trend. A sound estimate of the observed oxygen trends can hence be a powerful tool to constrain predictions of future changes in oceanic deepwater formation, heat and carbon dioxide uptake. Estimating decadal scale oxygen trends is, however, a nontrivial task and previous studies have come to contradicting conclusions. One key potential problem is that changes in the historical observation network might introduce considerable errors. Here we estimate the likely magnitude of these errors for a subset of the available observations in the Southern Ocean. We test three common data analysis methods south of Australia and focus on the decadal-scale trends between the 1970's and the 1990's. Specifically, we estimate errors due to sparsely sampled observations using a known signal (the time invariant, temporally averaged, World Ocean Atlas 2001) as a negative control. The crossover analysis and the objective analysis methods are far less prone to spatial sampling location biases than the area averaging method. Subject to numerous caveats, we find that errors due to sparse sampling for the area averaging method are on the order of several micromoles kg^{-1}. For the crossover and the objective analysis method, these errors are much smaller. For the analyzed example, the biases due to changes in the spatial design of the historical observation network are relatively small compared to the trends predicted by many model simulations. This raises the possibility to use historic oxygen trends to constrain model simulations, even in sparsely sampled ocean basins.

Key words : Temporal oxygen trends, Southern Ocean, Estimation errors, Climate change, Assessment of historical observation networks

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1. Introduction

Understanding the processes and sensitivities of the oceanic thermohaline circulation (THC) is crucial to understand past climate variability and to predict future climate change (Alley *et al.* 2003; Broecker 1997). Numerous model simulations suggest that anthropogenic greenhouse gas emissions may already have caused a slowdown of deepwater formation in the North Atlantic and the Southern Ocean (Cubasch and Meehl 2001). These model predictions are, however, uncertain (e.g., Latif *et al.* (2000) vs. Rutherford *et al.* (2003)). These uncertainties may be reduced by a careful analysis of observational constraints and a data-model intercomparison to pinpoint the potential need for model improvements. An analysis of decadal scale dissolved oxygen trends may be especially promising to reduce key uncertainties as the model simulations suggesting a significant weakening of the THC also predict substantial decreases in oxygen concentrations in the Southern Ocean over the past four decades (Matear *et al.* 2000; Plattner *et al.* 2002). As a result, the observational record of oceanic oxygen concentrations has the potential to constrain ocean circulation changes (Emerson *et al.* 2001; Keller *et al.* 2002). In addition, estimates of the current anthropogenic CO_2 budget hinge critically on the assumed steady-state (or the

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lack thereof) of the oceanic oxygen budget (Keeling and Garcia 2002).

Temporal oxygen trends in the oceans are driven by an intricate interplay between physical, chemical, and biological processes. Previous studies suggest four main mechanisms driving decadal scale oxygen trends: (i) changes in the ocean circulation, (ii) changes in oxygen solubility at the surface, (iii) changes in the remineralization fluxes of organic matter, and (iv) changes in isopycnic structure (Bindoff and McDougall 2000; Matear *et al.* 2000; Sarmiento *et al.* 1998; Shaffer *et al.* 2000). Consider, for example, the effects of a reduction in water ventilation rates. A water parcel leaving the ocean surface (in approximate equilibrium with the atmosphere for a given temperature and salinity) loses oxygen due to aerobic remineralization of organic matter (an oxygen requiring step). A decrease in ocean ventilation rates alone would hence cause a decrease in the subsurface oxygen concentrations, as it would decrease the importance of the oxygen sources (by advection) relative to the oxygen sinks (by respiration). Change in oxygen solubility (for example, by a warming of surface waters) would decrease the oxygen concentrations at which a water parcel "starts out" from the surface on its way to the oceanic abyss. Finally, an increase in the remineralization fluxes of organic matter would act to decrease the oxygen concentrations.

Attempts to detect the predicted oxygen trends in historical observations in the Southern Ocean have come to contradictory conclusions (e.g., Pahlow and Riebesell (2000) vs. Matear *et al.* (2000)). Pahlow and Riebesell (2000) report no discernible trend in apparent oxygen utilization (AOU) in the Southern Ocean. In contrast, Matear *et al.* (2000) report large and highly significant oxygen concentration decreases (as large as ~15 μmol kg^{-1}) between the Eltanin cruises (1960's) and WOCE transect (1990's) south of Australia (ca. 110-170°E, 50-60°S). The main differences between these two studies are the applied data-analysis methods and the analyzed regions. Pahlow and Riebesell (2000) use a "crossover analysis" of the entire Southern Ocean, while Matear *et al.* (2000) use a method that may be characterized as "area averaging" in a sub-region of the Southern Ocean. Here we test the hypothesis that errors due to changes in the historical observation network have contributed to this discrepancy. Note that the results of Pahlow and Riebesell (2000) are likely biased by several additional artifacts (e.g., the use of an isobaric reference frame or the long time horizon (Gruber *et al.* 2000; Zhang *et al.* 2000)) that are not a subject of this analysis. We focus on the problem that past estimates may not be robust with respect to methodological choices. Resolving this potential problem is an important step towards the use of oxygen trends as constraints on ocean circulation models.

The central question of this study is how robust are the estimated oxygen trends with respect to methodological choices? To address this question, we analyze dissolved oxygen observations from the World Ocean Atlas 2001 (WOA01) (Conkright *et al.* 2002b) sampled at the sparse historic observation network, World Ocean Database 2001 (WOD01) (Conkright *et al.* 2002a). Specifically, we extract the WOA01 oxygen data at the actual observation locations in the 1970's and the 1990's, and compare the differences using three different methods. The WOA01 is a time-averaged record. Any temporal trends resulting from the analysis steps using this record are hence an artifact of the method of the choice. This is, in a sense, application of a simple negative control for previously used data analyses steps.

2. Data

The available hydrographic observations over the last few decades in the Southern Ocean are quite sparse, more so than other oceans basins (Conkright *et al.* 2002a). In addition, the oxygen tracer field in the Southern Ocean is

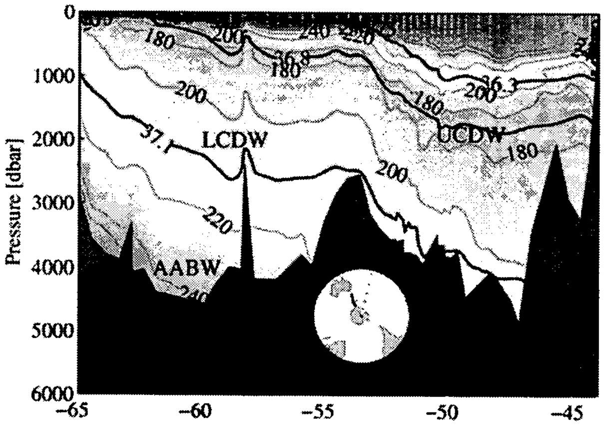

Fig. 1. Dissolved oxygen concentration section [μmol kg^{-1}] along the WOCE SR03 expedition observed in 1996 (Diggs *et al.* 2002). A few density (σ_2) layers are shown to delineate typical water masses in the Southern Ocean. UCDW, LCDW, and AABW denote Upper Circumpolar Deep Water, Lower Circumpolar Deep Water, and Antarctic Bottom Water, respectively. See inset for the geographical location.

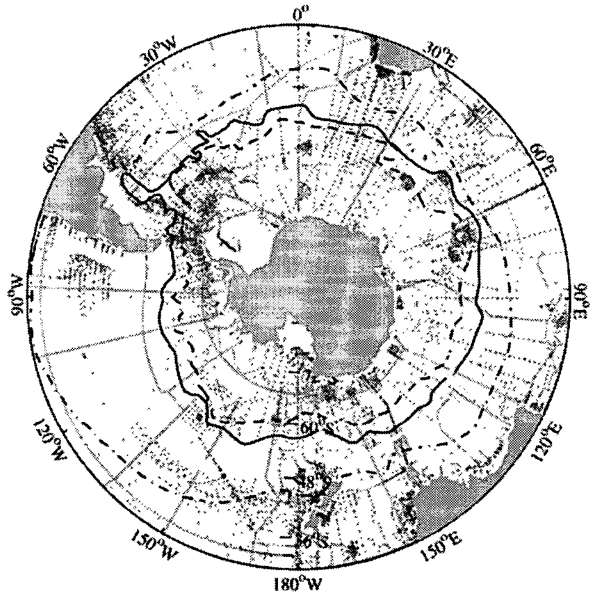

Fig. 2. Observation locations for oxygen in the 1990's (red) and the 1970's (blue) in the Southern Ocean (WOD01, Conkright *et al.* 2002a). The crossover locations (referenced to the 1990's locations) with a grid size of ±2° longitude ×1° latitude (green) between the two time periods are shown with squares. The analyzed region for the method intercomparison (110-170°E, 50-60°S) is outline by the yellow box.

highly variable depending on locations, depths, or water masses (see Fig. 1 for an example ocean section along WOCE SR03 which corresponds to the current study area). In this example, the depth of the oxygen minimum is over 1500 m north of 50°S along SR03 transect (see Fig. 1), shoaling abruptly to a few hundred meters below surface south of 60°S across the circumpolar current system. We choose the similar region as analyzed in Matear *et al.* (2000). Specifically, we analyze dissolved oxygen observations south of Australia between 110° and 170°E and 50° and 60°S for the time periods of the 1970's and the 1990's.

We estimate decadal-scale oxygen trends and the associated uncertainties by using the WOD01 data (Conkright *et al.* 2002a) (Fig. 2). World Ocean Database 2001 (WOD01) is a compilation of the ocean observation data obtained in the world oceans during the past several decades by many different groups and countries on various platforms with extensive quality flags (Conkright *et al.* 2002a). World Ocean Atlas 2001 (WOA01) is a time-average climatology database estimated with the WOD01 data by using multiple steps of data quality controls, statistics, and objective analysis (Conkright *et al.* 2002b).

3. Methods

We compare the ability of three different methods to recover the given (by definition) signal of zero temporal trend from the WOA01 data using information available in the historical observation network. The first step is to construct decadal scale averages for the 1990's and the 1970's. We remove questionable observations using the WOD01 quality flags. Furthermore, we remove obvious remaining outliers of temperature, salinity and oxygen data as additional quality checks. For the crossover analysis, we only use the oxygen data within the same isopycnal layer and within salinity difference less than 0.02, to reduce effects due to changes in water masses. We additionally limit the analysis to stations with oxygen observations below the climatologically mean (WOA01) wintertime mixed layer depth to reduce the effects of seasonal aliasing (as most observations in the Southern Ocean have been carried out during the austral summer seasons). We interpolate the time-averaged WOA01 oxygen data onto the actual historic oxygen observation locations (WOD01) and apply the three methods to the same data sets. We correct for the vertical location bias by comparing observations on common density (σ_2, potential density reference to pressure of 2000 dbar) coordinates. We aggregate the oxygen data for individual decades (i.e., 1970's with 1971-1980 data and 1990's with 1991-1998 data) to generate decadal average oxygen data sets. The temporal oxygen tracer trends are then the averaged recent observations (i.e., 1990's) minus the averaged historic observations (i.e., 1970's) at the same isopycnal. We calculate the mean trend for a given isopycnal surface and separately for each ocean basin (i.e., the Pacific, Atlantic, and Indian sector) and for each oceanic frontal zone (Orsi *et al.* 1995).

In summary, we use historic observations (i.e., WOD01) and climatological data (i.e., WOA01) south of Australia to explore methodological uncertainties in estimated decadal-scale oxygen changes derived by the techniques of: (i) "area averaging", (ii) "crossover analysis", and (iii) "objective analysis".

Area averaging method

The "area averaging" method estimates the mean oxygen concentrations in a certain time period and region (e.g., between the Subtropical front and Subantarctic front in the Pacific basin and the 1970's) for individual density intervals. The temporal change is then obtained by the difference between the 'averaged' estimates for two time periods. Matear *et al.* (2000) have applied this method to estimate the oxygen trend in the Southern Ocean south of Australia. This method assumes that all samples between fronts (or geographic boundaries) are from a single statistical population. As a result, this method is potentially quite vulnerable to sampling location biases due to spatial tracer trends (discussed below).

Crossover analysis method

The crossover analysis compares observations at close-by stations (e.g., within a 2° long. ×1° lat. box) visited at different times to estimate the changes from the differences of the values. This approach is well tested (Keller *et al.* 2002; Peng and Broecker 1984; Ross *et al.* 1999), and the method consists of conceptually straightforward and well-tested procedures. Unlike the area averaging method, the crossover analysis method uses only a subset of observations within the target region. This methodological choice hence compounds the data scarcity problem in the Southern Ocean, but has the advantage to correct better for the station location bias than the area averaging method. We compare close-by stations within ±2° × 1° and ±4° × 2° longitude by latitude regions referenced to the 1990's observation locations.

Objective analysis method

The third method to estimate oxygen trend applies the objective analysis algorithm (Bretherton *et al.* 1976; G. Johnson, personal communication) to the oxygen observations within two time windows for a certain layer (depth or density) and subtracts the two interpolation results. Previous studies (Keller *et al.* 2002; Garcia *et al.* 2003) using variants of this method show that the interpolation step can improve the signal-to-noise ratio of the estimated trends. The objective analysis method relies on a choice of a spatial correlation function and correlation length scale to represent the underlying tracer field (Bretherton *et al.* 1976). We derive a gridded estimate of the oxygen field by first removing the overall mean field and then by using the 128 closest observations to each grid point to derive an objectively weighted value. For each set of grid point and the 128 closest data points, their grid-to-data cross covariances are calculated using an exponential functional form. It is assumed that the correlations between data points depend only on the distance among them. We choose correlation length scales of 15° long.×7° lat. to approximate the earlier choices of 1550 km × 740 km used in the open oceans (R. Key, personal communication), and to consider an anisotropy effect. We do not analyze interpolated data with very large interpolation errors to avoid comparing unreasonable values.

4. Results and discussion

We present potential artifacts in estimating decadal-scale oceanic oxygen trends caused by using different analysis methods in a sub-region of the Southern Ocean. Estimates of decadal-scale tracer trends might be affected by (i) spatial sampling biases, (ii) temporal sampling biases, or (iii) analytical artifacts. This study focuses on spatial sampling biases due to temporal shifts in sampling locations. These shifts in the sampling locations alias spatial and temporal variability and introduce potential errors in the estimated trends. Second, temporal sampling bias may be introduced, for example, by seasonal aliasing in relatively shallow waters or by averaging over too long time periods (e.g., Pahlow and Riebesell 2000). These temporal biases can be reduced by excluding the more variable shallow water masses (Keller *et al.* 2002). Finally, the analytical biases are expected to be less important for long-time averages with a larger number of observation data, provided that a systematic offset is not so significant. If the analytical errors for a single observation or station were random, they would affect the large-scale trends only marginally. This is because the large-scale trends are derived from the combination of many observations on the order of hundreds or even thousands. For normally distributed and independent random errors, the approximated standard error of the mean trend would be relatively small (equal to the standard deviations of the n trend observations divided by $\sqrt{n}$). For example, if we assume such analytical errors in the oxygen measurements with a standard deviation of 5 μmol kg^{-1} (arguably a conservatively large estimate (WHPO 1994) and a random sample of 1000 stations, then the expected standard error of the mean would be less than 0.16 μmol kg^{-1}.

We estimate the standard deviation of all trends within the study region divided by the square root of the number of observations. This measure approximates the standard deviation of the mean trend reasonably well as long as the errors are statistically independent and identically distributed and follow a normal distribution. This approximation would be violated if the estimated trends are autocorrelated (Wilkes 1997). This autocorrelation would act to decrease the effective number of the degrees of freedom. As a result, the standard deviation of all trends divided by the square root of the number of observations would be an

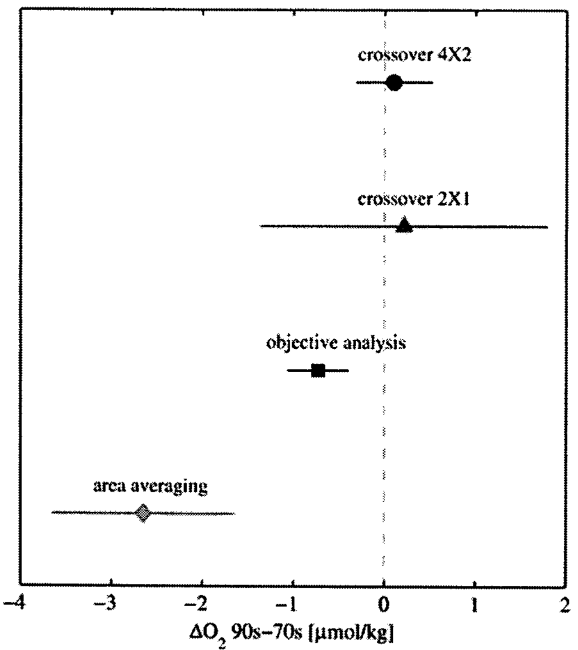

Fig. 3. Comparison of different estimation methods of oxygen changes in this region (110-170°E, 50-60°S, 36.80 ± 0.05 σ_2) using the WOA01 data at corresponding WOD01 observation locations in the 1970's and the 1990's. Dashed line denotes the true zero signal from the negative control test (i.e., no artificial temporal trend estimated by a method of choice) when using the time-average WOA01 data. The horizontal bars denote 1.96 times the standard deviation of all trends divided by $\sqrt{n}$ (see text for detail).

overconfident (i.e., biased towards too small values) measure of the error of the mean.

We choose a particular time interval (the 1990's vs. the 1970's), area (110°-170°E and 50°-60°S) and depth (the $\sigma_2 = 36.8$ isopycnal surface corresponds roughly to the layer of the Upper Circumpolar Deep Water (UCDW) or the oxygen minimum water in this part of the Southern Ocean, see Fig. 1) for this study. If there were no spatial sampling biases between the two time periods, the estimated results from all methods should converge to the true zero signal (dashed vertical line in Fig. 3) as we apply the analysis onto the same time-average data. In contrast, our analysis shows considerable trends for the different methodological choices, thus indicating potentially important artifacts due to changes in the historical observation network.

The area averaging method applied to the WOA01 data interpolated to the historic observation locations yields a trend estimate that is considerably biased (Fig. 3). The area averaging method yields a biased estimate with poor accuracy and a poor precision (filled diamond in Fig. 3). Accuracy is here defined by the difference between the estimated trend and the known true signal. We characterize the method precision by the approximated standard error of the mean (95% confidence interval in Fig. 3) for the estimated trend. The crossover analysis method with a relatively small comparison box size (i.e., ±2° × 1°, see filled triangle in Fig. 3) shows higher accuracy than the area averaging method, but still has a relatively poor precision (about ±2 μmol kg^{-1}). Comparing of small area in the ocean might be more vulnerable to effect of the temporarily changing small-scale ocean features (e.g., eddies), or individual data quality. The crossover method using a larger comparison box (i.e., ±4° × 2°, see filled circle in Fig. 3) shows an improved accuracy and precision (both within ~0.5 μmol kg^{-1}). We hypothesize that this improved accuracy and precision is due to a counterbalancing effect between the extent of allowed spatial oxygen gradient and the number of available crossover observations within the comparison box. Finally, the objective analysis method results in a quite reasonable accuracy and precision (see filled square in Fig. 3) that is comparable to a crossover analysis using the larger comparison box (i.e., ±4° × 2°). Overall, the crossover analysis and objective analysis methods are more accurate and robust than the area averaging technique in estimating decadal-scale oxygen trend in the Southern Ocean.

5. Conclusions

We compare different analysis methods for decadal-scale oxygen trends in the Southern Ocean south of Australia to demonstrate the influences of methodological choices on the estimated tracer trends. The area averaging, crossover analysis, and objective analysis methods are applied to the same data sets for comparison using WOD01 and WOA01 datasets. The crossover analysis and the objective analysis methods yield more accurate tracer trends than the area averaging method for the analyzed data set. Estimates of historic oceanic oxygen trends have to be carefully corrected for potential spatial sampling errors. The errors introduced by changes in the historical observation network are considerable, but can be estimated (and hence be corrected for).

Historic oceanic oxygen observations contain valuable information about the oceanic response to anthropogenic climate change. Utilizing this information requires a sound assessment of the errors in the observed trends introduced by the changes in the historic observation network. Our analysis suggests that a simple negative control can be used to estimate and to correct for these errors. This is an important step to address the question whether the observed trends are consistent with the fingerprints of reduced deepwater formation rates predicted by the model simulations. This will also shed more insights in resolving the discrepancy in interpreting oceanic oxygen trends by previous studies.

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