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Exposing XBT bias in the Atlantic sector of the Southern Ocean

K.A. Hutchinson [a,*], S. Swart [a,b], I.J. Ansorge [a], G.J. Goni [c]

[a] Department of Oceanography, Marine Research Institute, University of Cape Town, Rondebosch 7701, South Africa
[b] Southern Ocean Carbon and Climate Observatory, CSIR-NRE, PO Box 320, Stellenbosch 7599, South Africa
[c] NOAA/AOML/PHOD, 4301 Rickenbacker Causeway, Miami, FL 33149, USA

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ABSTRACT

Hydrographic data from three research cruises, occupying the GoodHope line in the Atlantic sector of the Southern Ocean, are used to identify and quantify Expendable Bathythermograph (XBT) temperature biases. A set of 148 collocated XBT and CTD stations, separated by a maximum distance of < 12.5 nm and < 10 h, are used in this study. A subset of these comparisons is also investigated.

This subset consists of 24 simultaneous pairs where the XBT and CTD stations are within 2.5 nm and 2 h of one another. These simultaneous pairs are extremely rare in XBT bias experiments and provide data set to assess, in deeper detail, the behaviour of the bias. The net bias, which is a product of both the depth offset and the pure thermal bias, is investigated with depth per frontal zone for both the collocated and simultaneous comparisons and found to be on the whole positive, meaning warmer XBT readings compared to the CTD values at each depth. The total mean bias for all collocated pairs was found to be 0.101 ± 0.024 °C, and for the simultaneous subset the net bias had a mean value of 0.130 ± 0.064 °C. An investigation into the magnitude of the depth offset was also undertaken, exposing generally positive depth biases, thereby indicating an overestimation of depth by the fall rate equation. A sizeable variation in bias between frontal zones is observed, along with an expected increase of net bias in regions of steeper temperature gradient. The contribution of the pure thermal bias is explored and found to be comparatively small yet still sizeable (mean bias $= 0.053 \pm 0.063$ °C). Results found in this study further support the hypothesis of the regional dependence of the XBT fall rate on water temperature, and thus water viscosity. In addition, results obtained here highlight the need to develop an XBT bias correction scheme specifically appropriate to the Southern Ocean.

1. Introduction

Expendable Bathythermographs (XBTs) were adopted by oceanographers in the late 1960s to obtain valuable upper ocean temperature profiles, and have since then made up the majority of the historical subsurface (to approximately 800 m depth) temperature data archive (Seaver and Kuleshov, 1982). With the recent development of more sophisticated equipment, measurements from other instruments have begun to dominate, however XBTs still remain popular and currently represent approximately 25% of all ocean temperature measurements (DiNezio and Goni, 2009). The historical XBT dataset has been used to investigate global change of the upper ocean heat content (Levitus et al., 2009; Gouretski et al., 2010). However, examinations of temperature profiles have shown that when compared to more accurate instruments (i.e. Conductivity Temperature and Depth profilers (CTDs), and Argo profiling floats) sizeable biases are found (Reseghetti et al., 2007; Gouretski and Reseghetti, 2010). The net bias of XBT instruments is thought to stem from two sources: a depth bias, and a pure thermal error (Hanawa et al., 1995; Gouretski and Koltermann, 2007; Gouretski and Reseghetti, 2010).

As XBT data are relatively dominant in the historical global ocean temperature archive, in particular during the 1970s to 1990s, the impact of these errors is sizeable and therefore of critical importance for climate-related studies (Wijffels et al., 2008). Biased temperature profiles may lead to erroneous estimates of ocean heat content variability, heat transport changes, and thermosteric sea level rise (Gouretski and Koltermann, 2007; Domingues et al., 2008; Wijffels et al., 2008; Ishii and Kimoto, 2009; Levitus et al., 2009). Uncertainties in ocean heat content variability estimates, as a result of uncorrected XBT data, may therefore result in the incorrect identification and quantification of the oceanic effects of climate change (Gouretski and Koltermann, 2007; Levitus et al., 2009; Hamon et al., 2012).

One of the core objectives of the Southern Ocean Observing System (SOOS) is to improve both the quality and quantity of ocean sampling (Rintoul et al., 2009). Recent observations that form part of the SOOS, have suggested that the Southern Ocean is

* Corresponding author. Tel.: +27829282752.
E-mail address: kath.hutchinson@gmail.com (K.A. Hutchinson).

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warming at a rate faster than the global ocean (Gille, 2008). However, as XBT data are relatively dominant in this region, it is unclear whether this warming signal is partly due to an artefact of biases in the data, or to an actual long-term climate change signal. It is, therefore, critical that the bias is correctly estimated in the Southern Ocean, in order to accurately assess the magnitude of variability in this region and to correct XBT temperature data accordingly.

The goal of this study is to present results from an investigation of the XBT bias carried out in the Atlantic sector of the Southern Ocean. The GoodHope line (or National Oceanic and Atmospheric Administration (NOAA) AX25 transect) is an established repeat sampling track between South Africa and Antarctica. This transect provides a unique opportunity to study this bias in a region characterised by pronounced horizontal temperature gradients. Results obtained here indicate the presence of a net bias in the XBT data for the region of the Southern Ocean south of Africa. This bias exhibits a geographical dependence related to the various frontal zones. The magnitudes of the depth bias and pure thermal error are also investigated. This work is organized as follows: Section 2 presents the XBT bias issue and Section 3 describes the data and methods used in this study. Section 4 addresses the results and provides a discussion: first for all collocated pairs, and then in a slightly more detailed exploration, for the bias associated with the simultaneous pairs, which are a subset within the collocated comparisons. Finally, Section 5 presents a conclusion to the findings.

2. Defining XBT bias

XBT bias studies (Hanawa et al., 1995; Gouretski and Koltermann, 2007; Gouretski and Reseghetti, 2010; Hamon et al., 2012) have shown that the XBT bias is comprised of two sources of error: a depth offset and a pure thermal bias (hereafter named T-bias). These two different sources of errors are very difficult to separate accurately and then assess their respective contributions to the net error. However, using the temperature-error-free method, it is possible to gauge the magnitude of the depth bias within each vertical layer of the water column (Hanawa and Yoritaka, 1987; Kizu et al., 2005, 2011). The size of the pure T-bias is estimated using regions of very small temperature gradient.

2.1. Depth bias

XBT depth is not measured directly using a pressure sensor, but is instead inferred from the time elapsed after the XBT makes contact with water, via a fall rate equation (FRE) that uses empirically-derived coefficients (Green, 1984; Hallock and Teague, 1992; Hanawa et al., 1995; DiNezio and Goni, 2009). The FRE is based on a simple dynamic model that takes into account the hydrodynamic features of the probe behaviour in water and the change in its characteristics (e.g. mass) with depth (Green, 1984; Hanawa et al., 1995). The fall rate equation provided by the XBT inventor and main manufacturer (Sippican Co., now Lockheed Martin Sippican) and that applies to the XBTs relevant to this study, is as follows:

$$Z = At - Bt^2,$$

where Z is the depth in meters and t is time in seconds since the probe hits water. The coefficients are empirical constants related to the physics of the probe descent and depends on the XBT type. Among the available versions of XBT probes, the most used and popular types are T4/T6 and T7/DB, all having the same values for the coefficients: $A = 6.472\ \mathrm{ms^{-1}}$ and $B = 0.00216\ \mathrm{ms^{-2}}$. The dynamics of the XBT fall however, are more complex than those implied by the manufacturer's FRE, indicating that the coefficients of the equation may not be appropriate (for example Hallock and Teague, 1992; Hanawa et al., 1995; DiNezio and Goni, 2009).

The equation presumes that the XBT fall rate is constant throughout all oceans. This is possibly flawed given the global differences in water mass properties. The speed of descent of the probe through the water column is a function of the viscosity of the water (Seaver and Kuleshov, 1982). Kinematic viscosity of seawater varies inversely to temperature, meaning that viscosity is highest in cold oceans near the poles, and lowest in warm tropical waters (Green, 1984; UNESCO, 1994; Boyer et al., 2010). The resultant effect of changing viscosity with geographical location, due to water temperature, is that the XBT manufacturers' equation may erroneously estimate depth in many regions (Wijffels et al., 2008). The inadequacy of the FRE is thought to be the largest source of error in XBT profiles (Hanawa et al., 1995; Gouretski and Koltermann, 2007).

The most popular and maybe most accurate method of calculating the depth offset was developed by Hanawa and Yoritaka (1987), and since used in many XBT bias studies. Arguably the most notable example of the implementation of this method is that of Hanawa et al. (1995) where new values for the coefficients of the FRE of T4/T6/T7/DB probes manufactured by Sippican and TSK are proposed. The usefulness of this methodology is that it unambiguously separates depth errors from pure T-errors (DiNezio and Goni, 2011). In essence, the temperature-error-free method uses the profile of temperature gradient (TG) to identify markers in the XBT profile and compare the depth of these features with the depth of the closest TG value in the CTD profile (Hanawa and Yoritaka, 1987). Over time, this method has been adapted and improved through the use of various filters on the data, and careful choice of the search window and range of each of the markers to ensure an even distribution of estimates along the entire profile (Hanawa and Yoshikawa, 1991; Hanawa et al., 1995; Kizu et al., 2005).

Alternative methods for diagnosing the depth bias component of the XBT error have also been utilized. For example, Good (2011) and Gouretski (2012), compared the maximum depth of XBT profiles against a bathymetry data set. For both studies, the General Bathymetry Chart of the Oceans (GEBCO) was used as a reference for bottom depth. The limitation of this method however, is that the XBT profiles used, were for shallow water areas, mostly near the coasts (Good, 2011; Gouretski, 2012). On the other hand, Cheng et al. (2010) proposed a method using integral temperature profiles instead of TG profiles, also including an offset term.

2.2. Temperature bias (T-bias)

Pure thermal error stems from instrumental bias, which arises from instability and discrepancies in different acquisition systems, transient effects within the surface layer, response time of the thermistor, launching conditions, and the inaccuracy of the temperature sensor itself (Kizu and Hanawa, 2002; Reseghetti et al., 2007; Gouretski and Reseghetti, 2010). Transient effects occur in the upper layer where quick thermal changes occur, as it takes some time for the probe to adjust to the temperature of the surrounding water (Reseghetti et al., 2007). The cumulative effect of all instrumental errors creates a pure T-bias. This T-bias is, however, thought to be small compared to the depth bias introduced by the unfit FRE and its coefficients (Reseghetti et al., 2007; Gouretski and Reseghetti, 2010).

2.3. Detection of the XBT bias

It has been widely accepted that the most effective and reliable way of assessing the extent of the bias, is to compare XBT-derived temperature measurements against those simultaneously made with more accurate CTD profilers (Anderson, 1980; Gouretski et al., 2010). CTDs have a combined temperature and depth accuracy of an order of magnitude greater than XBT specifications (Seaver and Kuleshov, 1982). The CTD temperature accuracy ranges from 0.003 °C to 0.02 °C, and the depth accuracy is approximately 2 m (Ishii and Kimoto, 2009). The manufacturers' specifications for all XBT types are a temperature error within 0.15 °C and depth accuracy of 2% of the depth, or 5 m, whichever is greater (Seaver and Kuleshov, 1982). However, the global accuracy of an XBT system is estimated to be ±0.2 °C. Generally CTD profilers are calibrated before and after each voyage and the results applied to the data before analysis (UNESCO, 1994). CTDs are therefore regarded as the "field standard" and so the CTD measurements are considered the true temperature profile, against which the XBT profile is compared to assess biases. Any differences derived from these comparisons are assumed to reflect a bias in the XBT measurements (Reseghetti et al., 2007). In order to correct for the bias in the global XBT data set, side-by-side comparisons with CTDs are therefore evidently necessary.

Previous XBT-CTD inter-comparison studies have rendered differing results. This may be partly due to the methodology used for the comparisons as the launching procedures and conditions are usually different from the standard operational conditions. In addition it may also be due to the dependence of the XBT fall rate parameters on viscosity, and thus water temperature, thereby rendering the XBT bias dependent on the region where the probe is deployed (Thadathil et al., 2002; Gouretski and Reseghetti, 2010). Results from Reverdin et al. (2009) show a correlation between bias and water temperature, as the bias was found to be larger for areas of high sea surface temperature. Thadathil et al. (2002) compared XBT-CTD pairs in Antarctic waters, and found that XBTs dropped in the Southern Ocean fall at a slower speed than those deployed in other areas. The unpublished cruise reports of Wisotzki and Fahrbach (1991) and Turner (1992) also mention a dependence of XBT bias on geographical area, but do not report conclusive findings. Boyer et al. (2010) concludes that the relationship of the XBT bias with ocean region is likely due to the influence of temperature on viscosity (first noted by Seaver and Kuleshov, 1982). Furthermore, it appears that the net bias is not just dependent on the viscosity (temperature) of the water, but also on the change in temperature with depth. Reverdin et al. (2009) found the largest biases in regions of maximum TG, with a local maximum usually at the thermocline. The major part of this bias in areas of steep TG is thought to be as a result of the depth bias, as the bigger the depth offset, the larger the net temperature error will be (Reverdin et al., 2009).

This net bias has been effectively identified and estimated in the tropical and subtropical oceans (Hanawa et al., 1995; Fang, 2002; Reseghetti et al., 2007). Conversely, the investigation of the descent of the XBT probes at high latitudes and remote oceanic regions has been somewhat deficient. There have been a few polar cruise reports that mentioned a deviation in XBT data when compared to CTDs, but no decisive conclusions were made (Pennington and Weller, 1981; Wisotzki and Fahrbach, 1991). Thadathil et al. (2002) performed an XBT comparison study from 16 stations in Antarctic waters and found both a positive depth and temperature bias in XBT data. However, thus far, an extensive investigation into the behaviour of XBTs in polar waters, especially the Southern Ocean, has remained largely absent.

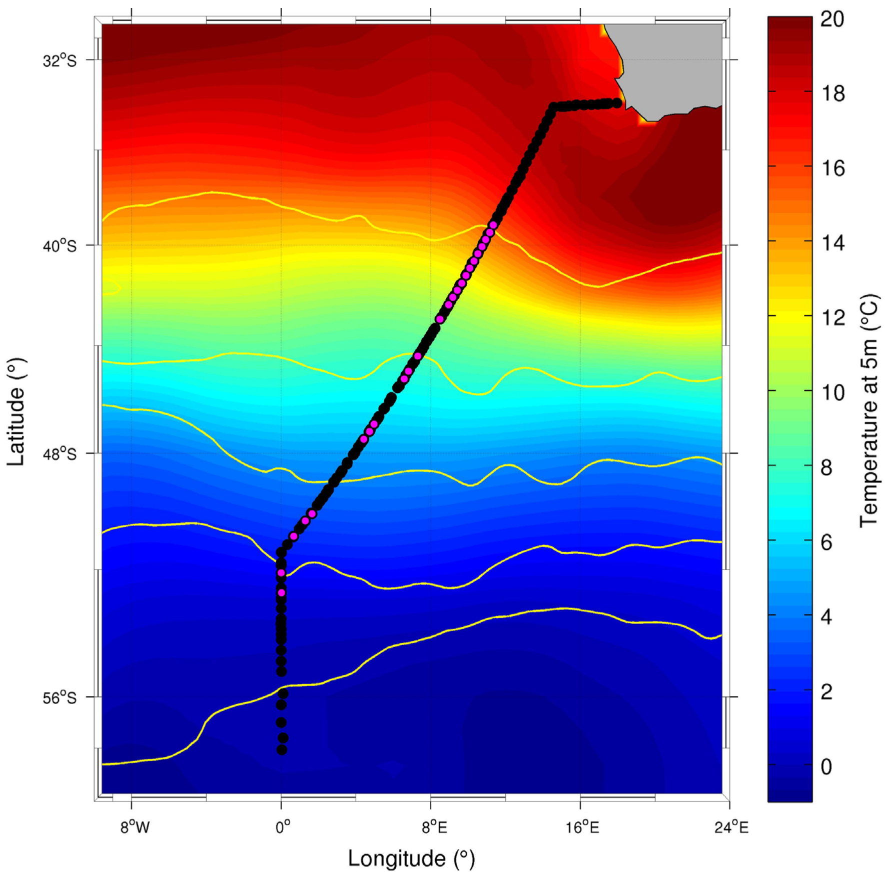

Fig. 1. Map showing location of all collocated stations (black dots) and the simultaneous stations (magenta dots) used in this study overlaid onto the mean observed temperature at 5 m (from EN3 Objectively Analysed dataset; Ingleby and Huddleston, 2007) for the region. The mean location of the ACC fronts determined using satellite altimetry (Swart et al., 2012) are depicted from north to south using yellow curves: STF, SAF, APF, SACCF, SBdy.

3. Data and methods

3.1. Data

XBT and CTD data collected from three GoodHope research cruises (Fig. 1) were used in this study. The first GoodHope section (hereafter referred to as GH2004) was completed in November 2004, and the second was occupied during October 2005 (hereafter referred to as GH2005). Both these sections were carried out by the Shrishov Institute of Oceanology, Moscow, Russia, aboard the Research Vessel (RV) Akademik Sergey Vavilov (Gladyshev et al., 2008; Swart et al., 2008). The International Polar Year cruise, which was undertaken in collaboration with the Bonus-GoodHope Program, took place in February–March 2008 (hereafter referred to as BGH2008). During this cruise, hydrographical sampling was performed aboard the RV Marion-Dufresne II.

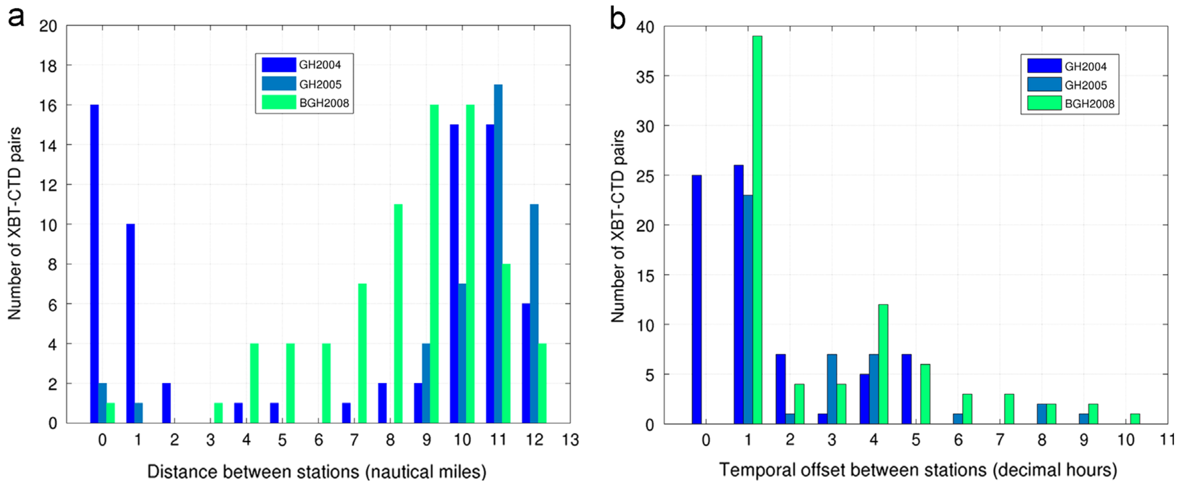

Fig. 2. (a) Histogram showing the number of XBT-CTD pairs that fall into each distance bin for the three cruises. (b) Histogram showing the temporal offset between the collocated XBT and CTD stations.

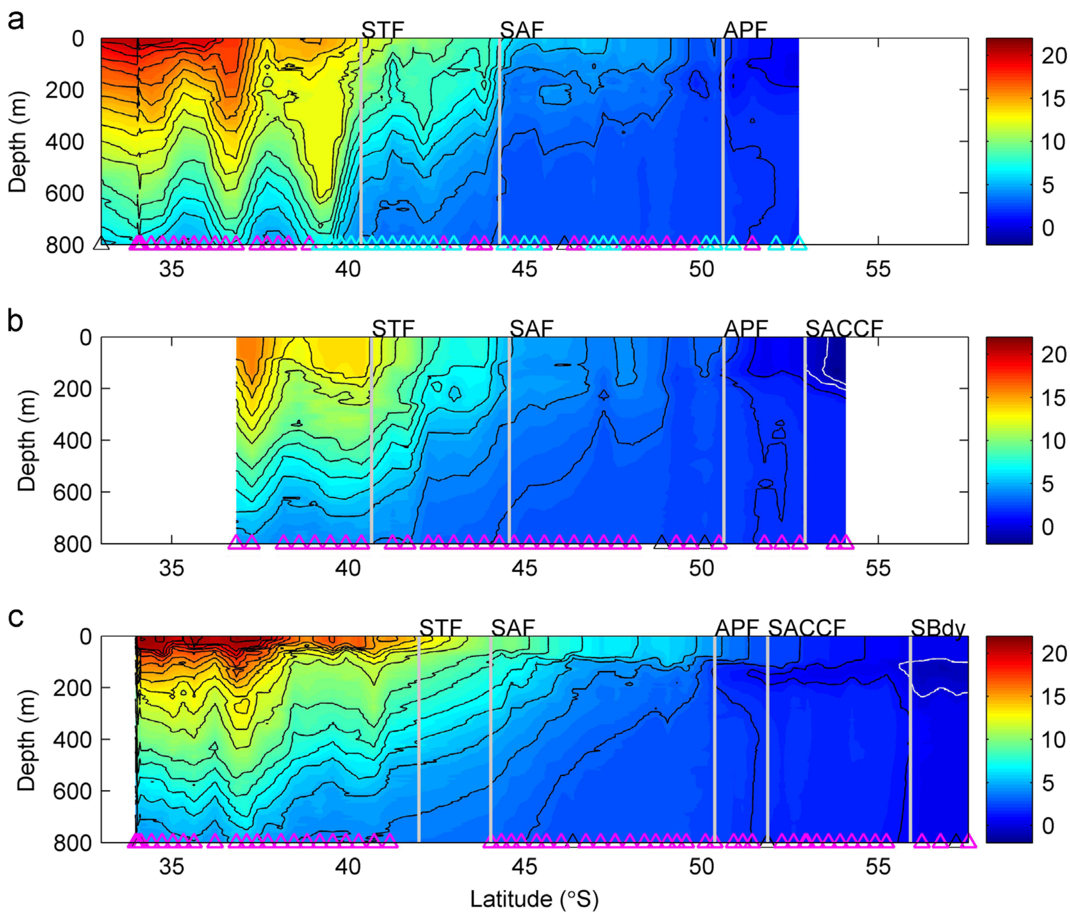

Fig. 3. Temperature sections for the (a) GH2004, (b) GH2005 and (c) BGH2008 crossings of the GoodHope line. The frontal positions identified for each cruise are overlaid and labelled. The positions of the collocated stations are shown as magenta triangles, and the simultaneous pairs are marked as cyan triangles. Isotherms are overlaid, black corresponding to all positive values, and the white isotherms indicating 0 °C and below.

The Lockheed Martin Sippican Deep Blue XBT was the only type of XBT deployed on all the three cruises and used in this study. An MK21 system was used with AMVERSEAS software. Even though the manufacturer's maximum depth for XBT Deep Blue probe is set at 760 m, most of the XBT probes deployed on the GoodHope occupations measured temperature to a depth of 800 m. Data acquisition beyond the nominal terminal depth is a procedure well known for XBT probes—without any evidence of reduced accuracy in the measurements (Reseghetti et al., 2007). Therefore profiles reaching a maximum depth of 800 m are used in the present analysis. From all three cruises, 148 XBT-CTD collocated pairs were identified (refer to Fig. 1). GH2004 is the only cruise for which a significant amount of contemporaneous comparisons (station pairs separated by <2.5 nm and <2 h) were available within the collocated pair group; therefore these 24 stations are referred to here as the "simultaneous pairs" (see location as magenta dots on Fig. 1).

The CTD system used a SEABIRD SBE911+ probe. The temperature readings obtained during the downcast of the CTD were considered the true temperature profile and used for the comparisons. The upcast profiles are thought to be unreliable as the water has been disturbed and somewhat mixed by the turbulence created by the CTD rosette during descent, and by bottle triggering resulting in stops during the ascent. The CTD temperature sections for each cruise can be seen in Fig. 3. These transects indicate the temperature ranges sampled during each of the cruises. Due to the XBT depth limitations, this study only makes use of the upper 800 m of CTD temperature and pressure data.

3.2. Methods

3.2.1. Qualification of XBT-CTD pairs

The sampling strategy of all three cruises used in this study was to space XBTs and CTDs 10 nautical miles (nm) apart when not performing a dual XBT and CTD station. The collocated pair category encompasses all pairs of XBT deployments and CTD stations within 12.5 nm of one another, which is the upper limit of the 10 nm bin. The cut-off of distances that fall into the 10 nm bin is set at 12.5 nm, as the intervals between CTD and XBT stations are often slightly larger than intended. In total, 53 stations fall into this category for GH2004, 33 for GH2005, and 82 for BGH2008, with the distribution for the BGH2008 cruise peaking at 10 nm (Fig. 2a). Combined, there are 148 XBT-CTD collocated pairs available for this study (before quality control).

Within the large category of collocated XBT-CTD pairs, a subset of 24 simultaneous comparisons was identified. Simultaneous comparisons apply to XBT-CTD pairs where stations fall within 2.5 nm and 2 h of one another (Fig. 2). These direct comparisons (magenta dots in Fig. 1) are therefore regarded as XBT-CTD stations that were performed at the same location and at the same time. The small spatial offsets between the locations of the XBT deployment and the CTD profiles (<2.5 nm) are mostly due to the drift of the ship during the CTD cast. The temporal offsets are regarded as an upper estimate, since CTD times were recorded at the start of the CTD descent, and XBTs were deployed just after the completion of the CTD cast. This indicates that in fact the temporal offsets between the CTD and XBT could be considerably less than those reported here. This procedure is somewhat unusual, as usually XBTs are deployed within few minutes from the launch of the CTD profiler in order to reduce the difference due to the ship drift during the cast. Simultaneous pairs are not common in XBT bias experiments, particularly at high latitudes, and thus the results obtained from these comparisons are extremely valuable. The collocation method used by Hamon et al. (2011) had a resolution of 1° latitude (60 nm), 2° longitude (120 nm) and 15 days between XBT and CTD stations. Reverdin et al. (2009) had XBT and CTD stations separated by on average 50 km (~27 nm) and 3–4 h. In comparison, the simultaneous pairs used in this study can reasonably be viewed as having a negligible spatial and temporal gap between XBT and CTD profiles. Therefore any offset in XBT measurements can be considered a direct product of the inherent bias.

3.2.2. Data quality control

For all stations within the collocated pair category, it was critical to verify that the pairs were not situated over oceanic fronts or eddies, where steep horizontal TGs may mean that the two profiles could represent the sampling of different water masses, and thus lead to an unrealistic reported bias. An oceanic front marks the interface of two water masses and therefore indicates an area of sharp TGs. Within the region of the Southern Ocean, south of Africa, five established fronts are found: the Subtropical Front (STF), Subantarctic Front (SAF), Antarctic Polar Front (APF), Southern ACC Front (SACCF), and the Southern Boundary (SBdy) of the ACC (Orsi et al., 1995). The front locations were determined using the criteria of Orsi et al. (1995) for each cruise (see Fig. 3 for the respective frontal locations), and any XBT-CTD stations located directly over a front and were discarded. The same procedure was followed when evident ocean eddies (such as Agulhas Rings found in the northern part of the section) were sampled.

Occasionally a single XBT was close to more than one CTD (within the 12.5 nm collocated offset limit). The CTD station with the shortest distance to the XBT was therefore kept, and any other proximate station discarded to avoid weighting the influence of that single XBT too largely on the reported bias for the whole cruise. The histograms shown in Fig. 2 represent the number of stations per cruise before the quality control procedure (some of these stations were removed if they fell into the above mentioned criteria).

If conditions were particularly windy and rough seas were experienced, the copper wire of the XBT occasionally made contact with the ship's hull, thus inducing a spike in the temperature profile. Insulation failure of the copper wire may also produce spikes in the XBT profile. The measurements made at depths deeper than the spike often appear accurate; however, they are likely to be erroneous (Anderson, 1980). For all XBT data used in this study, the spikes and all temperature values below the spikes were discarded. The probes were thermalized outdoors prior to deployment, in order to avoid thermal shock resulting in erroneous measurements in the surface layer. The Atlantic Oceanographic and Meteorological Laboratory (AOML), as part of NOAA in the United States, have undertaken extensive quality control procedures regarding the XBT data. The reliability of XBT profiles was evaluated, compared to adjacent profiles and to the climatology of the region from Levitus (1982). For more information on the AOML quality control procedures, refer to Bailey et al. (1994) and Daneshzadeh et al. (1994).

3.2.3. Net bias analysis

The depth of the XBT was calculated from the time elapsed using the equation provided in Section 2.1, and the XBT data subsequently interpolated onto a 1 m vertical grid during on-board data acquisition. The CTD measured depth in decibars, and therefore the pressure reading was converted to depth as a function of latitude for each station. The CTD data was then interpolated to every 1 m of depth so that direct comparisons could be made with the XBT data. The upper 2 m of temperature data for each XBT profile was excluded, as this is where the XBT is often known to report inaccurate data due to thermal shock and transient effects in the surface layer (Reseghetti et al., 2007). As

800 m is the accepted maximum depth of the XBT Deep Blue probe, 798 depth levels were identified with a 1 m interval.

The net bias was calculated for each 1 m level for each station, by subtracting the CTD temperature value from the XBT temperature measurement at that same depth. In order to produce a robust estimate of the bias dependence on ocean temperature (water mass properties) and geographical location, the Southern Ocean fronts were used to demarcate different frontal zones. Bias profiles within these zones may be grouped together as they signify the response of the XBT error to the same water column structure and characteristics. The frontal boundaries used to divide up the stations are shown in Fig. 3. The mean net bias with depth from all comparisons within that zone was then obtained, along with the total mean for all collocated pairs (all zones), which is also reported.

3.2.3.1. Depth bias. The depth offset was calculated using the temperature-error-free method originally developed by Hanawa and Yoritaka (1987). The first step of the process is the filtering of the data to remove small-scale geophysical and instrumental noise. The filtering was performed according to the procedure outlined by DiNezio and Goni (2011), where the XBT and CTD profiles that are already interpolated onto a 1 m vertical resolution are smoothed using a second order Butterworth filter with a 5 m low pass cut off. Next the temperature gradients (TGs) were calculated per 1 m from the filtered profiles. The top 30 m was excluded from the depth-offset analysis according to Kizu et al. (2005). This layer is more or less coincident with the depth needed for the probe to be situated within the conditions required by the standard FRE. The depths of the maximum and minimum TGs in the XBT profile were selected as the markers (Hanawa and Yoshikawa, 1991). These markers were identified for every 25 m layer so as to ensure an even distribution of markers over the entire profile. In order to obtain the depth of the most similar feature in the CTD TG profile, a window originally centred at the depth of the XBT marker was moved up and down the CTD TG profile searching for the TG value closest to that of the XBT marker (Hanawa et al., 1995; Kizu et al., 2011). The full search span of this window is 50 m, 25 m above and 25 m below (Kizu et al., 2005). The depth difference between the XBT TG marker and the corresponding closest TG value within the search window of the CTD TG profile gives the depth offset, calculated as XBT depth minus CTD depth. For both collocated and simultaneous comparisons, the depth offset with depth is presented averaged from all pairs in each frontal zone. As the water mass properties within each zone are similar, it is not incorrect to average results within these geographical segments.

3.2.3.2. Pure thermal bias. The relative contribution of the pure T-bias to the net bias is thought to be small (Gouretski and Reseghetti, 2010). It is, thus, somewhat difficult to isolate the magnitude of the T-bias due to the relative dominance of the depth bias. In thermally homogenous areas, however, it is not possible to identify the XBT depth bias as there are no identifiable changes in vertical gradients in the temperature profiles (Wijffels et al., 2008). Therefore, we use these areas of low vertical TG to gauge the size of the T-bias. The bias was averaged for all areas where dT/dz is less than 0.002 °C/m (criterion according tom Hamon et al. (2011)) to give an approximation of the T-bias.

4. Results and discussion

4.1. Collocated pairs

4.1.1. Net bias

The collocated pairs (XBT-CTD stations separated by <12.5 nm and <10 h) were divided up into zones according to the fronts defined for each cruise shown in Fig. 3. In total, 55 station pairs were located north of the STF, 20 between the STF and SAF,

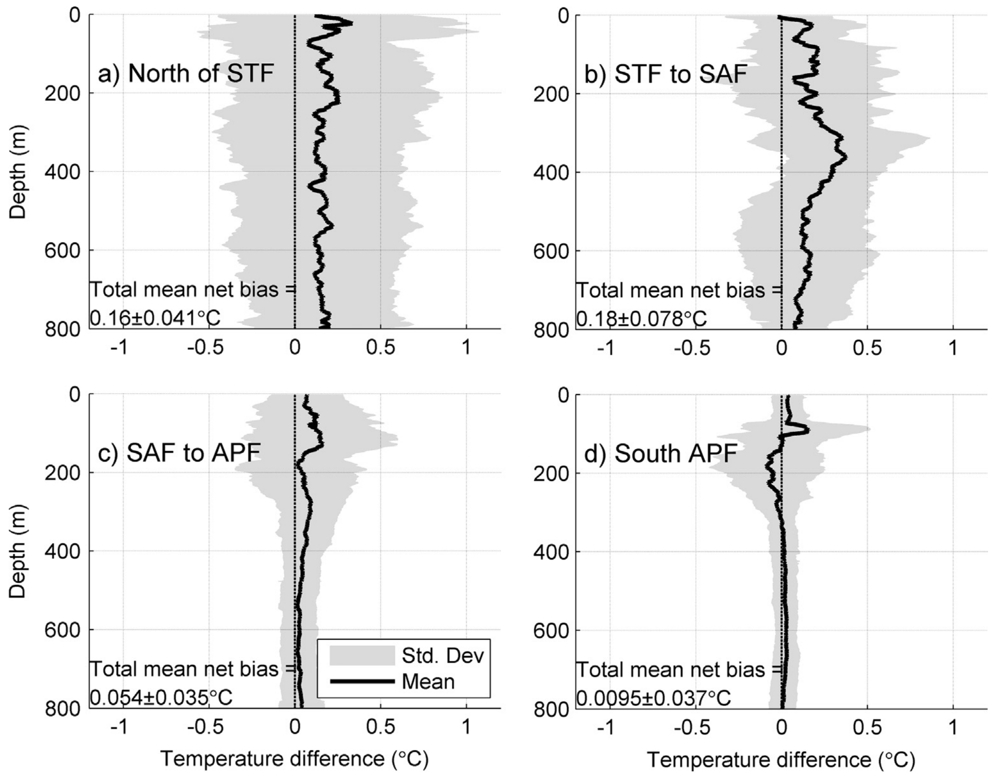

Fig. 4. The mean net temperature bias with depth for collocated comparisons is shown as a solid black line, with standard deviations of mean bias shaded in grey for each frontal zone (a)–(d). The total mean bias and standard deviation for each zone is reported.

49 from the SAF to APF, and 28 south of the APF. Fig. 4 indicates that the net bias is positive at all depths for the northernmost 3 zones, and even though south of the APF the mean bias is seen to become negative between ~150 m and ~300 m, the total mean for this region is still positive.

A positive (negative) bias signifies that XBT system is recording warmer (colder) values at each depth compared to the CTD readings. Throughout all frontal regions, the net bias is large in the upper portion of the temperature profile, where the TGs increase over the mixed layer depth interface/thermocline. These results are in agreement with those obtained by Reverdin et al. (2009), where the net bias was also found to be on average positive, with a maximum of just under 1 °C at approximately 100 m depth (see Fig. 3 of Reverdin et al., 2009).

North of the STF where TGs are steep over the entire uppermost 800 m (as can be seen in Fig. 3), the net bias is consistently large, always positive and without significant variability with the depth (Fig. 4a). The results pertaining to the region between the STF and SAF (Fig. 4b) show an interesting elevated bias within the depth range 300–400 m depth, with a maximum at ~380 m. This is perhaps due to a deeper mixed layer in this area. However, it is important to note that all stations from BGH2008 within this zone were removed due to the presence of a large Agulhas ring, thereby reducing the sample size in this segment. The average value of the bias in this region is of similar magnitude to that the zone to the north of STF, however with a much higher variance. The net bias profile for the zone between the SAF and APF shows a large positive bias in the top 150 m and a small bias below this depth (see Fig. 4c). Once again the larger bias correlates with the steep vertical gradients of the upper layer. The zone south of the APF presents an unusual net bias profile (Fig. 4d). The hypothesis behind the negative bias maximum around 200 m is the presence of a sub-surface temperature minimum layer of Winter Water (discussed in Section 4.2.1.1 in greater detail). The average net biases in the regions between SAF to APF, and south of the APF, are smaller than those belonging to the other two regions and the values are dominated by the differences in the upper parts of the profiles. Therefore, there is a big standard deviation, despite the fact that the bias values at deeper depths are very small. As the collocated pairs are separated by a maximum offset of 12.5 nm and 10 h, the results from these pairs, while interesting, are less reliable than those from the simultaneous comparisons. The standard deviations of the mean bias with depth are relatively large, reflecting the sizeable variance in calculated bias amongst individual collocated stations and between the three cruises used in this assessment. We therefore discuss the variation of bias with geographical location in deeper detail in Section 4.2.1.1, as the simultaneous pair results can be considered more dependable.

4.1.1.1. Source of the net positive bias. The greatest contributor to the largest values of this overall positive bias may be attributed to the shortcomings of the FRE to accurately compute the depth of XBT temperature measurements. The FRE provided by the Sippican Deep Blue XBT manufacturer applies to all ocean regions ranging from the warm, salty tropics to the cold, fresh Antarctic domains. We hypothesize here that the higher viscosity of cooler water masses in the Southern Ocean may induce more drag on the XBT probe (Seaver and Kuleshov, 1982), therefore resulting in a slower rate of descent. A slower-than-estimated fall rate of the XBT probe results in temperature readings being shallower than the reported depth, leading to considerably warmer conditions than CTD readings at the same depth. We conclude here that this effect contributes significantly to the mean positive net biases seen in Fig. 4a–d, where the total mean bias over all zones is large and positive with a value of 0.101 ± 0.024 °C.

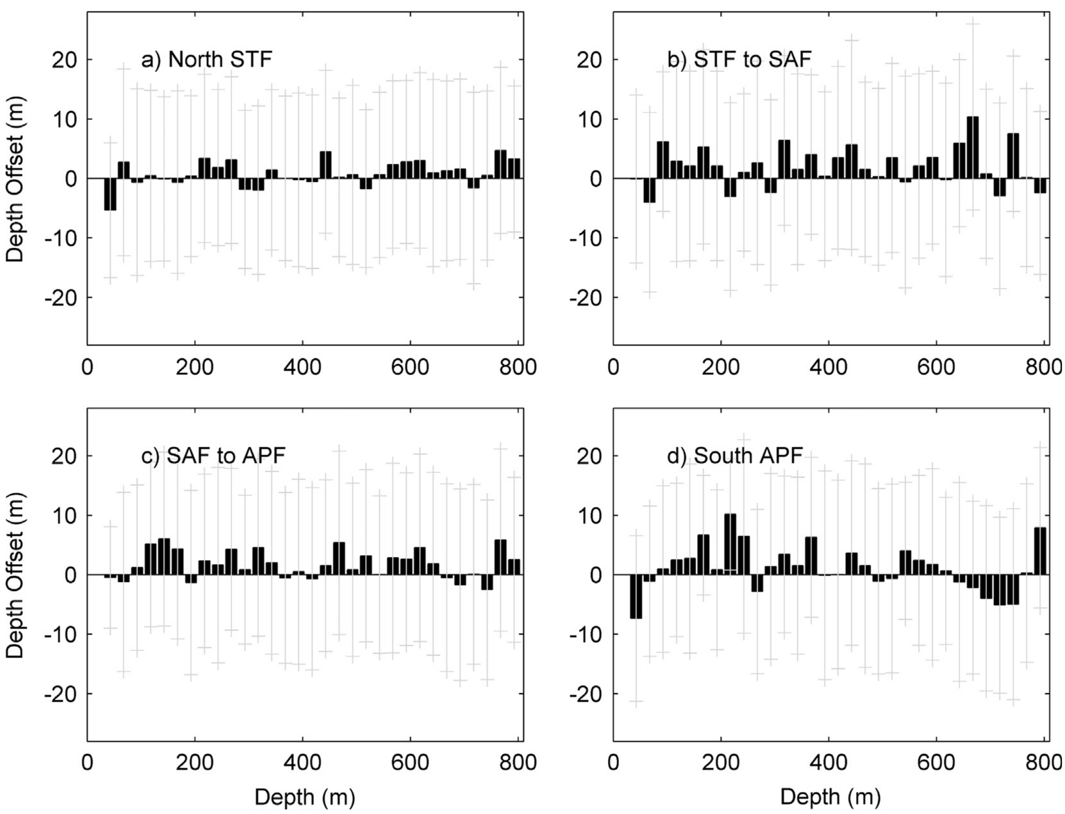

Fig. 5. Mean depth offset for each 25 m depth layer for the collocated comparisons. Standard deviations are marked in grey for each frontal zone (a)–(d).

4.1.2. Depth bias

In order to test the hypothesis suggested above (i.e. that the depth offset is significant), the mean depth bias with depth is assessed for each frontal region (Fig. 5). The depth bias is found to be positive at most depths. These results are similar in sign and magnitude to those shown in Fig. 3b of Reverdin et al. (2009). A positive depth bias supports the hypothesis that in colder and more viscous Southern Ocean waters, the XBT falls at a rate slower than that estimated by the manufacturers' FRE, resulting in an overestimation of reported depths. However, results shown here (Fig. 5) indicate that the depth offset occasionally exhibits negative values. A negative depth bias means that the TG marker identified in the XBT profile is at a shallower depth than the same TG feature identified in the CTD profile. There appears to be no clear pattern in the distribution of negative depth biases except that they are more prevalent in the region south of the APF (Fig. 5d). This may be an artefact of the fact that the region has very small vertical TGs and thus the features used as markers in the TG profiles are not very robust. It is important to keep in mind that for collocated stations, there may be a distance offset of as much as 12.5 nm, resulting in the possible sampling of dissimilar water masses.

4.2. Simultaneous pairs

In total, for the simultaneous pairs, 4 stations are located north of the STF, 9 between the STF and SAF, 8 between the SAF and APF, and 3 south of the APF. The simultaneous pairs, as a sub set of the larger collocated pair category, have a much smaller spatial and temporal difference between stations, and therefore the results obtained from their analysis can be considered more reliable. These comparisons (<2.5 nm and <2 h apart) present a rare and highly valuable database with which to evaluate the XBT biases. The contemporaneous comparisons are therefore used to investigate in further detail the behaviour of the net bias with frontal zone and TG, the depth error, and the possible contribution of the pure T-bias.

4.2.1. Net bias

Results from Fig. 6 indicate that on the whole, the net bias is largely positive for the direct comparison pairs. The total mean net bias over all frontal zones is sizeable with a value of 0.130 ± 0.064 °C. This indicates that at each depth calculated by the XBT FRE, the recorded temperature values are warmer than those reported by the CTD, likely due to an overestimation of depth by the FRE. The standard deviations of the mean net biases are overall smaller for the direct comparisons than for the collocated stations: an expected result, since the errors that may be introduced due to spatial differences between pairs are reduced. The implications of this positive net XBT bias on Southern Ocean heat content estimates are likely substantial, due to the relative dominance of XBT data in this region.

4.2.1.1. Variation in net bias per frontal zone. Past studies have reported a relationship between XBT bias and geographical area (Wisotzki and Fahrbach, 1991; Thadathil et al., 2002; Reverdin et al., 2009). Boyer et al. (2010) indicated that the relationship of bias with ocean region may be due to the influence of temperature on viscosity, which is fundamental in determining the probe motion. In order to investigate this, the net bias profiles were grouped into the different frontal zones. Water mass characteristics are similar within a frontal zone, but change dramatically between zones. Fig. 6a–d show net bias with depth profiles for the four frontal regions identified in the Southern Ocean south of Africa. The mean bias is largest in the STF-SAF frontal zone, with a mean bias of 0.21 ± 0.11 °C (Fig. 6b), and the area north of the STF (Fig. 6a) coming close in magnitude with an average error of 0.19 ± 0.13 °C. In the northern sector of the GoodHope line, the temperature decreases

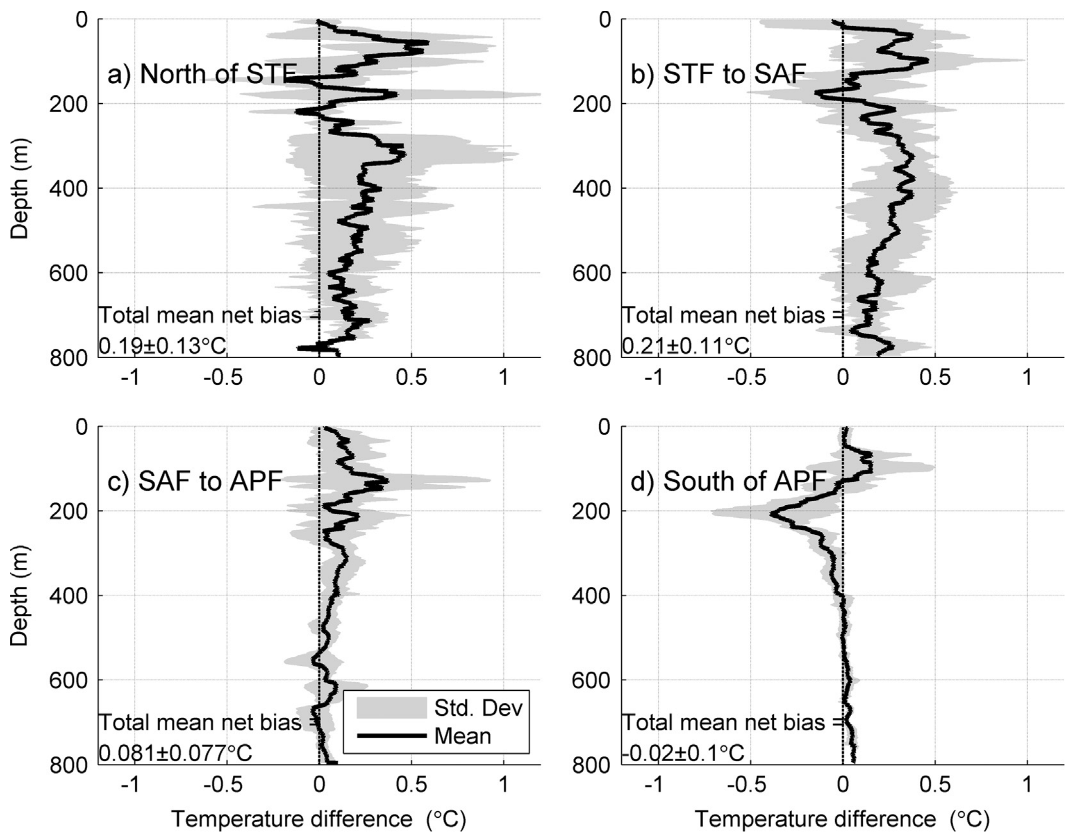

Fig. 6. The mean net temperature bias with depth for simultaneous comparisons is shown as a solid black line, with standard deviations of mean bias shaded in grey for each frontal zone (a)–(d). The total mean bias and standard deviation for each zone is reported.

markedly with depth (see Fig. 3), hence a slower fall of the XBT probe leads to shallower and significantly warmer readings than those of the CTD at the reported comparison depth. This situation produces the large positive biases seen in the northernmost two zones. The smallest bias found corresponds to the negative mean error belonging to the region south of the APF with a value of -0.02 ± 0.10 °C (Fig. 6d), where the variance is mainly due to strong variability in the upper 300 m. The bias profile of this region is particularly interesting due to the large minima in bias at 200 m depth. In this area, a subsurface temperature minimum exists (see isotherm pattern south of APF in Fig. 3), below which the temperature increases slightly with depth. This feature is associated with the presence of Winter Water, where temperatures average 2–3 °C cooler than the surface waters (Park et al., 1998). This feature is significantly accentuated in late summer when solar heating further separates the temperature minimum layer from the stratified surface layer. As a result of this temperature minimum layer, an XBT temperature reading that corresponds to a position higher up in the water column than the comparison CTD temperature reading will actually be lower in value than the CTD measurement. As the net bias is calculated by subtracting the CTD value at a depth from that measured by the XBT, this Winter Water layer produces a negative net bias.

Results presented here indicate that the net bias varies significantly with frontal zone and thus latitude; a concept that has never been so clearly observed or reported. Consequently, these results highlight the importance of correctly computing temperature measurements for estimating global ocean temperature trends. These results show that on average, the XBT probe falls at a rate slower than that estimated by the manufacturer's FRE throughout the colder, more viscous Southern Ocean waters. This effect supports the hypothesis of a different and slower fall motion of XBT in cold ocean conditions. However, a general decrease in bias with increasing latitude is in fact counter to the expected effect of the higher viscosity of these cooler waters. Therefore it is important to stress that the rate of descent of the XBT probe does decrease with colder temperatures. However, the implications of this statement vary depending on the structure of the water column. The observed net XBT bias (largely resultant from fall rate errors) is positive if temperature decreases with depth, negative if there is a vertical increase in temperature, or even zero if there is no vertical TG. There may also be a lag between the point where the XBT fall rate deviates from that predicted by the FRE, and where the effect of this deviation is manifested in a bias. The bias at a certain depth is not entirely a direct reflection of the water properties at that location, but seems to be rather a combined effect of the water characteristics at that depth, of the layer of water that the probe has just travelled through, and of the different dynamical and electrical responses of the XBT probe to such a variation.

A variation in bias with geographical location has been observed to some extent in previous studies. Hanawa et al. (1995) showed significant variation in XBT error results from different ocean areas and attributed these to the influence of viscosity and density on the XBT fall rate. Thadathil et al. (2002) noted that the bias results in the Antarctic Ocean are different from those in other regions. Gouretski and Reseghetti (2010), Figure 12a showed a warm bias at high latitude (cold water temperature), yet from their Figure 12d the low percentage of profiles available for the high southern latitudes is evident. This is true in general, as only one other XBT bias study has been undertaken in the Southern Ocean—that of Thadathil et al. (2002) with only 16 XBT-CTD pairs used in their study. Therefore, even though other studies have observed some variation in XBT bias with geography, none have done so as clearly as is presented in this study.

4.2.1.2. Relationship between net bias and TG. The largest contributors to the positive observed net bias are likely the errors associated with the erroneous depth estimated by the employed FRE. However, a lag time in instrument response may also have a non-negligible effect. In Fig. 6, throughout all zones, the mean net bias is largest in the top 200 m where vertical temperature changes are steeper. Therefore, in this section the hypothesis that the thermistor of the XBT probe experiences difficulty recording rapid changes in temperature with depth is tested. Theoretically, in areas of steep TG, the net bias should be seen to be largest. At any depth, the net bias (with the depth offset having the largest contribution to this value) will be proportional to the vertical TG at that level. Therefore, the depth bias may remain unchanged, but the net offset will increase in response to an elevated vertical rate of change in temperature. Fig. 7 confirms this hypothesised relationship between net bias and TG. The figure shows the mean net temperature bias for each value of TG. The total mean relationship between net bias and TG, over depth and the entire GoodHope transect, is represented by the trend line which shows that the bias increases on average by 0.0125 °C per 0.002 °C/m increase in vertical TG. The authors would, however, like to re-iterate that the contribution of TG to the magnitude of net bias at a certain depth is not fully a direct result of the actual vertical gradient at that point, but rather also a product of the structure of the entire water column above that depth. Therefore, the effects of a steep change in temperature may only manifest themselves in an elevated bias some meters below.

4.2.2. Pure thermal bias

The errors that are involved in the conversion of time elapsed to depth using the FRE, thereby creating a depth bias, are thought

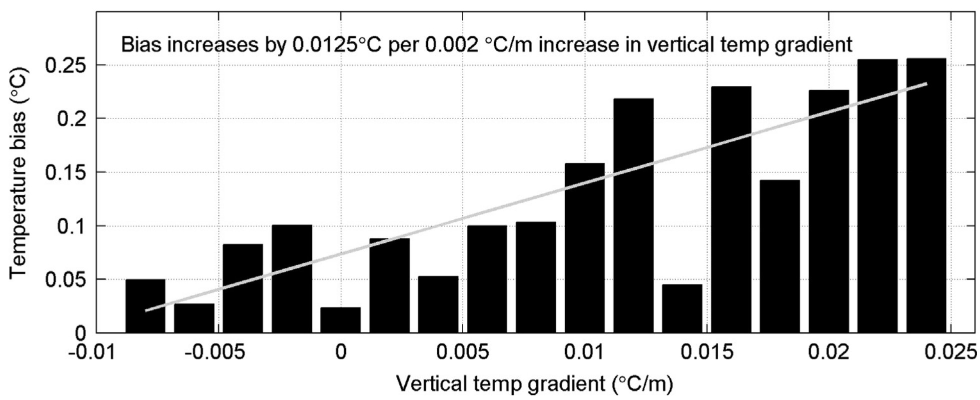

Fig. 7. Relationship of net temperature bias with the vertical temperature gradient. The trend in the bias with vertical change in temperature is marked as a grey line, and the rate of change reported.

to be the largest contributors to the net bias. However, in thermally homogenous regions, the depth bias of the XBT probe cannot be detected as the TG is near zero (Wijffels et al., 2008). We can therefore use these areas of low vertical TG to gauge the size of the pure T-bias, which is expected to be comparatively minor (Reseghetti et al., 2007). As the pure T-bias stems from instrumental error, it is likely that this bias is constant throughout the data. Here we have only investigated areas of low TG as these regions enable us to examine the pure T-bias without the dominating effect of the depth bias obscuring our estimates. The bias was therefore averaged for all areas where dT/dz is less than 0.002 °C/m (criteria specified by Hamon et al. (2011)) to give an approximation of the T-bias. This component of the bias was found to be very small, 0.053 ± 0.063 °C. The magnitude of this T-bias is comparable to the biases found by Hamon et al. (2011), where before 1980 the T-bias in deep XBTs was at a maximum with an average of 0.04 °C, and rose again in the 1990s to reach an average of 0.047 °C between 1995 and 2005. DiNezio and Goni (2009) identified biases in XBT data using Argo observations and satellite altimetry, revealing a positive T-bias of 0.07 °C for XBT data within the upper mixed layer. On the other hand, comparisons performed in a calibration bath indicated a difference in agreement with such results (see Gouretski and Reseghetti (2010)).

4.2.3. Depth bias

The depth-offset stems from the inaccurate conversion of time elapsed since the XBT makes contact with seawater, into depth, using the FRE. The FRE has fixed coefficients that remain unchanged for all ocean regions. However, the speed of descent of the XBT varies with location depending on the drag imposed on the probe due to the water viscosity (Seaver and Kuleshov, 1982). The largest contribution to the overall net bias, is thus likely the under or over- calculation of depth by the FRE (Boyer et al., 2010).

The depth bias was calculated using the temperature-error-free method described in Section 3.2.3.1. XBT markers were identified for every 25 m layer, and compared to the depth of the most similar CTD TG value within the search window. The depth-offset estimates are therefore available for every 25 m layer (excluding the top 30 m) of the XBT temperature profile. Fig. 8a–d shows the depth differences with depth for each of the frontal zones. Over the majority of depths for the northern 3 zones, the depth offset is sizeable and positive. One would expect an increase in depth bias with depth due to the compounded effect of the inadequacy of the manufacturer's FRE, which was used for all XBTs investigated in this study. However, this theoretical result is not clearly observed. At many depths, the reported depth offset is negative, and flanked above and below by a large positive depth offset. The ambiguity of these results suggests that more inter-comparison pairs are needed to better understand the behaviour of the depth bias with frontal region. If all simultaneous pairs are grouped together, and the depth difference averaged for each layer, the vertical profile does show a trend of an increase of depth bias with depth. However, as it is not advisable to group together results from regions of significantly different water mass characterises, this finding in not graphically depicted in this study.

The generally positive depth offset (seen in Fig. 8) supports the hypothesis that in cold, more viscous, Southern Ocean waters, the XBT falls at a rate slower than that estimated by the manufacturers' fall rate equation, resulting in an overestimation of reported depths. A fortiori, the use of the FRE coefficients proposed by Hanawa et al. (1995) has given rise to differences that are even more significant. As the depth error is thought to dominate the net XBT bias, many studies have proposed revised FREs to combat the problem (Hanawa et al., 1995; Gouretski and Reseghetti, 2010; Hamon et al., 2011). However, a revised FRE is not presented here, as more XBT-CTD simultaneous pairs are needed before an adequate FRE with accurate coefficients can be proposed for the waters of the Southern Ocean.

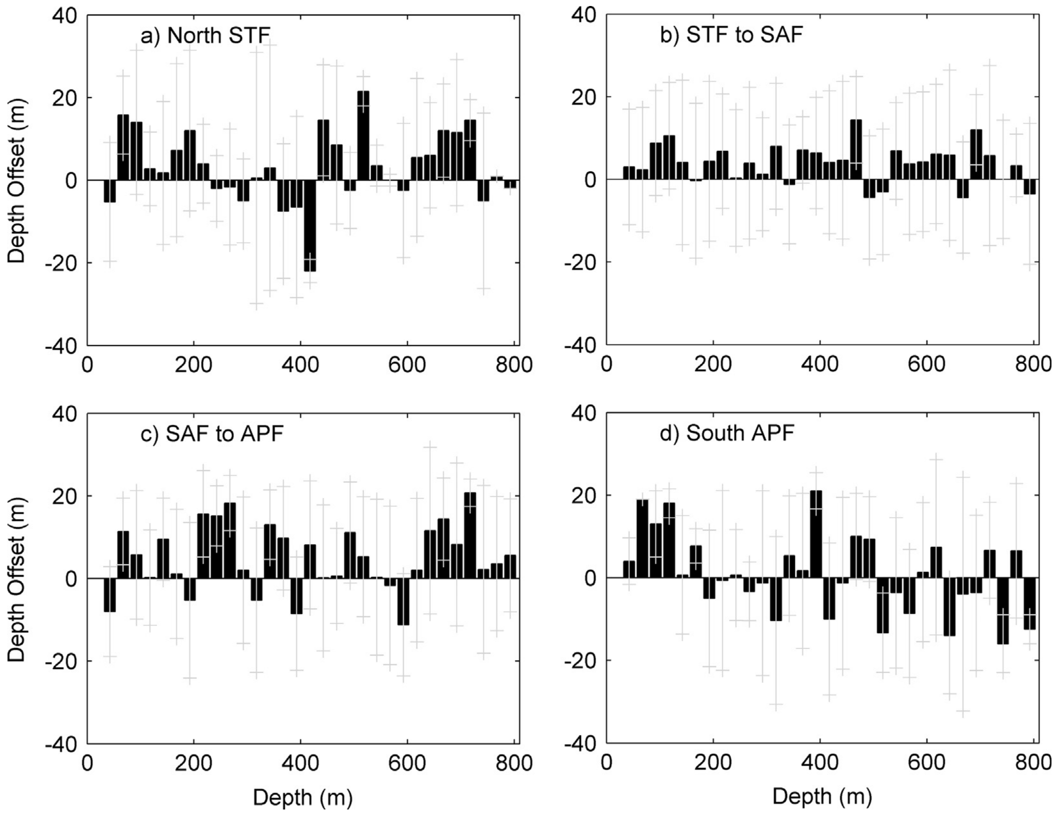

Fig. 8. Mean depth offset for each 25 m depth layer for the simultaneous comparisons. Standard deviations are marked in grey for each frontal zone (a)–(d).

5. Conclusions

This study examines the bias associated with XBT data obtained in the Atlantic sector of the Southern Ocean from three research cruises that occupied the GoodHope line between 2004 and 2008. In agreement with the results from an earlier study (Thadathil et al., 2002), which was also performed in the Southern Ocean, the XBT data was on the whole found to be overestimating depth and thus producing a positive net bias in the temperature data. Significant variation in net bias between frontal zones was observed, exposing the need to address this problem in XBT profile correction schemes. The sizeable magnitude of the net biases identified in this work, highlights problems associated with XBT measurements for climate studies. These results indicate that the real Southern Ocean warming may not be as pronounced as XBT time series indicate.

XBT data forms a large portion of the historical global temperature record, in particular during the 1970–2000 period. Studies such as this one will contribute to improve the accuracy and reliability of this record. In addition, XBTs continue to be very valuable as they are largely used to monitor the variability of boundary currents and fronts and provide approximately 10 to 15% of the upper ocean thermal observations along fixed transects and in regions that are highly under-sampled by other observing platforms. A better understanding of the errors associated with the XBT FRE will greatly help to assess upper ocean thermal variability and dynamics where XBTs are still a significant source of data. It is therefore critical to develop an appropriate correction scheme for this valuable record of upper ocean temperature measurements before using the data to estimate topical long-term changes in the thermal structure of the upper ocean.

Additional Southern Ocean XBT-CTD inter-comparison pair studies will be needed so as to understand better the behaviour of the XBT bias, its link with latitude, and to assess the relative contributions of each source of error to the net bias. These results are highly valuable to numerical modelling efforts to ensure accurate forcing, especially for climate relevant applications. Results presented in this study also highlight the importance of these inter-comparison efforts during GoodHope research cruises. In order to increase the number of simultaneous comparisons in this region of the Southern Ocean, all future GoodHope occupations will have XBTs launched simultaneously with CTD casts, Underway CTD operations, and profiling float deployments where possible. These additional observations and inter-comparisons studies will address a key objective of SOOS by improving sampling strategies and data accuracy. A deeper knowledge of the real uncertainties in XBT measurements, and their variations since the beginning of the use of XBT probes, is required and strongly recommended in order to correctly understand the response of the Southern Ocean to climate variability and change.

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