Reducing biases in XBT measurements by including discrete 1 information from pressure switches 2 Marlos Goes^{1,2,*}, Gustavo Goni², and Klaus Keller^{3,4} 3 1 Cooperative Institute for Marine and Atmospheric Studies, University of Miami, Miami, FL, 4 5 USA 6 2 Atlantic Oceanographic and Meteorological Laboratory, National Oceanic and Atmospheric Administration, Miami, FL, USA 7 3 Department of Geosciences, Penn State University, State College, PA, USA. 8 4 Earth and Environmental Systems Institute, State College, PA, USA. 9 10 Accepted in JTech – Final version 11 November 6, 2012 12 13 14 15 16 17 *Corresponding author: Marlos Goes, Cooperative Institute for Marine and Atmospheric Studies, 18 Rosenstiel School of Marine and Atmospheric Science, University of Miami, 4600 Rickenbacker 19 Causeway, Miami, FL, 33149, email: mgoes@rsmas.miami.edu and marlos.goes@noaa.gov.

21 Abstract:

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23 Biases in the depth estimation of expendable bathythermograph (XBT) measurements cause considerable errors in oceanic estimates of climate variables. Efforts are currently underway to 24 improve XBT probes by including pressure switches. Information from these pressure 25 26 measurements can be used to minimize errors in the XBT depth estimation. Here we present a 27 simple method to correct the XBT depth biases using a number of discrete pressure measurements. We use a blend of controlled simulations of XBT measurements and co-located 28 29 XBT/CTD data along with statistical methods to estimate error parameters, and optimize the use 30 of pressure switches in terms of number of switches, optimal depth detection, and errors in the 31 pressure switch measurements to most efficiently correct XBT profiles. Our results show that given the typical XBT depth biases, using just two pressure switches is a reliable strategy for 32 33 reducing depth errors, as it uses the least number of switches for an improved accuracy, and 34 reduces the variance of the resulting correction. Using only one pressure switch efficiently 35 corrects XBT depth errors when the surface depth offset is small, its optimal location is at middepth (around or below 300 m), and the pressure switch measurement errors are insignificant. If 36 37 two pressure switches are used, results indicate that the measurements should be taken in the lower thermocline and deeper in the profile, at approximately 80 m and 600 m, respectively, with 38 a RMSE of approximately 1.6 m for pressure errors of 1 m. 39

40

42 **1. Introduction**

The use of expendable bathythermograph (XBT) measurements started in the 1960's and rapidly 43 became a preferred observational device for measuring upper ocean temperatures due to their 44 ease of deployment and low cost, outnumbering the mechanical bathythermographs (MBTs) in 45 the 1970's and the Conductivity-Temperature-Depth (CTD) in the 1990's (Gouretski and 46 Koltermann, 2007). XBT observations account for a large percentage of the existing global 47 48 ocean temperature record (Ishii and Kimoto, 2009), and are likely to still be utilized for many decades, despite the emergence of newer oceanic observing technologies. 49 The XBT probe has a streamlined body, comprised of a heavy metal nose, plastic triangular fins 50 and a wire spool. When the XBT is dropped from a vessel, water flows past a thermistor through 51 52 a cylindrical hole in the nose. The water temperature changes the thermistor resistance, 53 producing a voltage response, which is captured on board the vessel and translated into a 54 temperature measurement (Georgi et al., 1980; Green, 1984). Since the XBT probe does not 55 contain pressure sensors, its depth estimate relies on a semi-empirical quadratic relationship between time of descent and depth, known as the fall rate equation (FRE): 56

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$$Z = at - bt^2, \tag{1}$$

which converts the time elapsed t (in seconds) since the probe hits the water to a depth Z (in meters). The FRE depends on two parameters, *a* and *b*, which account for the characteristics of the probe, as well as of the environment (Hallock and Teague, 1992; Green, 1984). According to the manufacturer (see Hanawa et al., 1994), the maximum tolerance for systematic errors associated with these depth estimates are typically $\pm 2\%$ of depth linear bias, a depth offset of \pm 5 m, and a temperature accuracy of $\pm 0.2^{\circ}$ C.

64	Recent studies (e.g., Wijffels et al., 2008) have shown that, for the historical XBT record, the
65	magnitude of the depth error could be greater than 3% at 800 m, and that these errors may be
66	dependent on the probe type and manufacturing year (Wijffels et al., 2008; Ishii and Kimoto,
67	2009; Gouretski and Reseghetti, 2010; Gouretski, 2012). Positive temperature biases are found in
68	both MBT and XBT temperature measurements, but XBT biases may account for most of the
69	apparent interannual variation of heat content in the ocean (Gouretski and Koltermann, 2007).
70	This greatly affects the reliability of climate models in simulating the effect of heat uptake by the
71	ocean, and, as a result, affects climate projections (e.g., Forest et al., 2002; Urban and Keller,
72	2009; Olson et al., 2012).
73	As a comparison, typical CTD measurements (e.g., Sea-Bird SBE 911) have a nominal accuracy
74	of 0.001 $^{\circ}$ C, and a nominal depth resolution of 0.015 m. Despite the fact that such values are
75	given for ideal conditions, and that the actual CTD precision may vary (see Boyer et al., 2011),
76	CTD measurements are perhaps the best standard for a "true" temperature record. Several studies
77	have analyzed the temperature errors of XBTs by comparing XBT measurements with co-located
78	CTD measurements (e.g., Flierl and Robinson, 1977; Heinmiller, et al., 1983; Hallock and
79	Teague, 1991; Kizu and Hanawa, 2002; Reseghetti et al., 2007). Historically, the temperature
80	gradient method has been the most widely used. By comparing the temperature gradients with
81	depth (dT/dz) of a CTD profile with those from an XBT profile, the XBT depth bias can be
82	corrected by finding vertical lags of maximum correlation and estimating stretching terms to be
83	applied to the XBT depth (Hanawa and Yoritaka, 1987; Hanawa and Yasuda, 1992). Other
84	methodologies have also been successfully applied for XBT profiles correction, such as the
85	technique proposed by Cheng et al. (2011), where the integral temperature instead of the
86	temperature gradient seems to improve on the temperature gradient method considerably.

Moreover, such a technique intrinsically requires an offset depth term. True thermal biases in 87 XBTs may also be estimated after the depth correction (DiNezio and Goni, 2011, Cowley et al., 88 89 2012), but this also requires information from a co-located CTD profile along the entire depth of the XBT profile. Results from previous studies (e.g., Levitus et al., 2009, Gouretski and 90 Reseghetti, 2010) indicate that thermal biases were generally higher, between 0.1-0.2°C from the 91 92 60's through the 80's, and decreased later on, stabilizing after 2000 at around 0.05° C. The FRE is highly dependent on many parameters, such as the viscosity of the water, the height 93 94 of the launch, and the state of the ocean where the probes are deployed. Parametric uncertainty in 95 the FRE is the biggest contributor for temperature biases in XBT measurements. Supplementary information could be used to constrain the XBT depth estimates: for instance, the addition of 96 97 pressure switches inside the probe could potentially reduce depth biases without a considerable price increase. Pressure switches are small resistors that are activated at certain depths during the 98 probe descent, marking those depths in the profile with spikes. These spikes are filtered during 99 100 post processing, and their depths are recorded and used to correct depth biases in the profile. Here, our goal is to investigate if future measurements from pressure switches will be able to 101 appropriately correct XBT depth biases. To this end, we derive an efficient and practical 102 103 approach that improves on current methodologies by not requiring the use of collocated CTD 104 profiles.

This manuscript is outlined as follows. In Section 2 we define the two datasets used in this study. In Section 3 we derive the methodology for the correction of the XBT depth biases using pressure switches, and the two statistical methods used to optimize the correction. In Section 4, we use simulated temperature profiles to test the capability of this correction with respect to (i) the number of switches and (ii) the errors in the pressure switch measurements. Additionally, we

use co-located temperature profiles to test the capability of the method on actual data, and (iii)
estimate the optimal depths for triggering the switches. Finally, in Section 5 we discuss the main
results of this study, including advantages and caveats of using pressure switches.

113

114 2. Data

115 We use two types of data in the present study: (a) climatological temperature profiles, and (b)

shipboard co-located temperature XBT/CTD profiles. These two datasets and their application in

117 the present study can be described as follows:

a) The experiments with simulated data are based on typical temperature profiles from the World

119 Ocean Atlas climatology product (WOA09; Locarnini et al., 2009), which consist of gridded data

with a $5^{\circ} \times 5^{\circ}$ horizontal resolution and 27 vertical levels. For the purpose of this study, we use

data from the upper 700 m of the ocean, interpolated linearly onto a 10 m vertical resolution.

b) The experiment with co-located data uses XBT and CTD observations collected in the tropical

123 North Atlantic during the PIRATA Northeast Extension 2009 (PNE09) cruise (DiNezio and

124 Goni, 2011). We selected 19 paired XBT and CTD casts deployed within 24 hours and ~10 km

apart. The selected XBT probes are the Sippican T7 manufactured in 1986, which are the probes

that showed the highest overall depth error in this dataset (DiNezio and Goni, 2011). The

original Sippican FRE coefficients ($a = 6.472 \text{ m s}^{-1}$ and $b = 216 \text{ x} 10^{-5} \text{ m s}^{-2}$) are used to estimate

the XBT depth (Z_{XBT}).

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130 **3. Methodology**

131 **3.1 Errors in XBT measurements**

132	Simultaneous XBT-CTD experiments (e.g., Flierl and Robinson, 1977; Hanawa, 1995; Thadathil
133	et al., 2002) have shown that the manufacturer FRE parameterization may be inadequate to
134	produce unbiased temperature data in the upper ocean. We illustrate the effect of an inaccurate
135	FRE parameterization on the 0-700 m global ocean heat content anomaly (OHCA) by simulating
136	a linear depth bias time variability as a sinusoidal with amplitude of 2% of depth (Figure 1).
137	OHCA is calculated globally using the WOA09 annual climatology (see Section 2a for data
138	description), and assuming that 50% of the global profiles are randomly affected by a common
139	depth bias. The global effect of the XBT depth biases in this simulation generates OHCAs with
140	amplitude on the order of 8 x 10^{22} J, which is the same order of magnitude as the observed global
141	OHCA linear trends since the 1960's calculated in Domingues et al. 2008 (~16 x 10^{22} J) and in
142	other recent studies (e.g., Levitus et al., 2009; Ishii and Kimoto, 2009), therefore complicating
143	the detection of human induced trends in ocean heat uptake.
144	In general, XBT-derived temperature profiles are affected by several sources of error (see for
145	example, Cheng et al., 2011). We have chosen to focus on four sources of errors in our analysis:
146	1) Pure temperature errors (T_0): These are remaining temperature errors after XBT depth
147	correction. These errors can be introduced by several factors, including probe-to-
148	recording device, (static) calibrations in laboratory, wire de-reeling, and leakages, most
149	of which producing a positive temperature bias (Cook and Sy, 2000; Reseghetti et al.,
150	2007; Gouretski and Reseghetti, 2010). The manufacturer temperature error is on the
151	order of 0.2°C (Hallock and Teague, 1992; Ishii and Kimoto, 2009, Gouretski and
152	Reseguetti, 2009), and we use this value as a constant temperature offset.
153	2) Inaccurate FRE parameterization (z_d , z_2): This is the pure FRE error. z_d is defined as a
154	linear depth bias given as a percentage of depth (Seaver and Kuleshov, 1982). We use z_d

155 = 3% of depth as a typical value of this parameter, which is in agreement with previous studies (e.g., Wijffels et al., 2008), and slightly higher than the manufacturer specification 156 of 2%. z_2 is a quadratic bias term, and is related to an acceleration term in the FRE 157 (Cowley et al., 2012). We consider this term $z_2 = 1e^{-5} m^{-1}$, which alone generates an error 158 of ~ 5 m at 700 m depth, and is in agreement with the estimates of Hamon et al. (2011) 159 160 and Cowley et al. (2012). 3) Depth bias (z_0) : This error arises from surface phenomena such as wave height 161 variability, entry velocity and angle of the probe (e.g., Abraham et al., 2012). In this 162 manuscript we use z_0 as a constant depth offset, typically $z_0 = 5$ m (Gouretski and 163 Reseghetti, 2010). 164 4) Random errors (ε_z , ε_T , ε_p): These errors affect all measurements, due to small variations in 165 the mean state of the environment, and also to the precision of individual probes (Georgi 166 et al., 1980). Here we approximate the random errors by a Gaussian distribution N(0, σ_i^2) 167 with mean zero and standard deviation σ_i . We distinguish three types of random errors, 168

169 for depth (ε_z), temperature (ε_T), and pressure (ε_p).

The typical values of the parameters used here are summarized in Table 1. Formally, we treat the four classes of XBT errors described above as deviations from an "error-free profile", which represents a CTD profile. Therefore, the depth of the XBT profile (Z_{XBT}) is the depth of the errorfree CTD profile (Z_{CTD}) plus the total depth errors (E_Z):

$$Z_{XBT} = Z_{CTD} + E_Z, \qquad (2a)$$

and the total temperature errors in XBT measurements (E_T) are defined similarly:

$$T_{XBT} = T_{CTD} + E_T , \qquad (2b)$$

177 where T_{XBT} and T_{CTD} are the XBT and the error-free temperature profiles, respectively.

178 The error components E_z and E_T are structured as follows:

179
$$E_Z = z_0 + z_d Z_{CTD} + z_2 Z_{CTD}^2 + \mathcal{E}_Z$$
(3a)

(3b)

$$E_T = T_0 + \mathcal{E}_T \quad .$$

In simulating discrete pressure switch measurements, additional contributions to the total errors arise from random errors (ε_p) in the pressure measurements themselves. Therefore, a certain pressure measurement P is decomposed as:

$$P = P_{CTD} + \varepsilon_p \tag{4}$$

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186 **3.2** Correction of the XBT measurement biases using pressure switches

Having defined the XBT errors analytically, we now derive a correction to the XBT profile using 187 188 pressure switch information. This correction is performed in two steps, (1) by first identifying the errors E_Z and E_T in equation (3a, b) and (2) subtracting them from the profiles. For this, we 189 assume that *n* pressure switch measurements (P_n) are performed during the descent of the XBT 190 191 probe through the water column (Figure 2), and the locations of these measurements $(Z(P_n))$ provide information about the correct depth of the profile. The correct depth of the XBT profile 192 (Z_{CORR}) is then given by an operational fall rate equation estimate (Z_{XBT}) minus a depth 193 correction *F* which is a function of the pressure measurements: 194

195
$$Z_{CORR} = Z_{XBT} - F(Z(P_n)).$$
(5)

Equation (5) is a continuous function of depth, but in practice it relies only on the discrete
locations of the pressure measurements. Using equations (2a) and (5), we derive the function F at
the *n* discrete locations as:

199
$$F(Z(P_n)) = (Z_{XBT_n} - Z(P_n)) = z_0 + z_d Z(P_n) + z_2 Z^2(P_n).$$
(6)

The reconstruction of the entire corrected profile depth (Z_{CORR}), which is known at discrete locations $Z(P_n)$, is performed by isolating $Z(P_n)$ from the second and third terms in equation (6), making it dependent on Z_{XBT} and the error parameters.

The degrees of freedom of the correction are determined by the number of pressure switches to be used. For $n \le 2$ switches and/or when the quadratic term (z_2) in Equation (6) is ignored, we apply a linear correction. For $n \ge 3$ and $z_2 \ne 0$, we use a quadratic correction.

Z_{CORR} is calculated as follows:

207 (i) Linear correction (n ≤ 2 switches or $z_2 = 0$): Solving the linear version of equation (6), we 208 have:

209
$$Z_{CORR} \approx Z(P_n) = \frac{Z_{XBT}}{1 + z_d} - \frac{z_0}{1 + z_d}.$$
 (7)

This approach is considered an unbiased estimator for quasi-linear errors and accurate pressure measurements. If only one pressure switch (n = 1) is installed in the XBT probe, we assume that $P_1 = P_{XBT_1}$, i.e., the pressure estimated at the initial depth of the XBT profile P_{XBT_1} is measured by a virtual pressure switch at the surface for calculation of the correction terms. (ii) Quadratic correction ($n \ge 3$ switches and $z_2 \ne 0$): The quadratic version of equation (6) produces a corrected depth according to:

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$$Z_{CORR} \approx Z(P_n) = \frac{-(1+z_d) + \sqrt{(1+z_d)^2 + 4z_2(Z_{XBT} - z_0)}}{2z_2}, \quad (8)$$

which takes into account only the positive sign of the square root to allow compensation between the two terms on the right side of Equation (8), and therefore limiting to a finite root value for small values of z₂.

Note that for the approaches (i) and (ii) to be applied, depth is first converted to pressure to simulate the pressure switch measurements, and later the corrected pressure profile is converted back to depth. We adopt the Saunders (1981) algorithm for the conversion between depth and pressure, which does not account for temperature and salinity effects on the pressure in the water column, and presents an average error of 0.1 m. For a number of *n* pressure switches, the parameters z_0 , z_d and z_2 are calculated using a least squares regression with *n* points. After the depth correction, the pure temperature bias can be determined by the average residual

227 temperature in the profile:

228
$$T_0 = \frac{\sum_{k=1}^{K} (T_{XBT}^k - T_{CTD}^k)}{K}.$$
 (9)

As in previous studies (e.g., Flierl and Robinson, 1977; Gouretski and Reseghetti, 2010),
equation (9) can only be applied to collocated temperature profiles.

231

3.3 Optimization methods for determining switch number and location

233 The method described in Section 3.2 applies for *n* pressure switches. The estimation of the

number of switches and the depths at which they are triggered during the probe descent is an

optimization problem. We use two optimization methods: (a) a "brute force" Root Mean Square
Error (RMSE) minimization is applied to simulated profiles as a sensitivity test for different
number of pressure switches and different sets of errors, and (b) a global optimization algorithm
for a likelihood maximization is applied to co-located XBT/CTD data to determine the triggering
depth of the pressure switches.

a) RMSE minimization of simulated data

241 These idealized experiments use simulated profiles based on the temperature profiles from the 242 WOA09 annual climatology. The original climatological profiles are considered error-free CTD 243 observations, whereas the XBT observations are simulated by adding typical errors to the original profiles. We simulate measurements of one to five pressure switches distributed 244 245 randomly along the XBT profile, and analyze three different cases, each of them using a different 246 set of errors in the simulated XBT profiles. In order to sample a large number of possible 247 combinations of the pressure switch locations, we select 12,500 random realizations of the 248 positions of the switches and random errors.

The accuracy of the FRE correction by pressure switch measurements is evaluated at a given combination of location of pressure switches using the root mean square error (RMSE), defined as:

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$$RMSE = \sqrt{\frac{\sum_{k=1}^{K} (Z_{CORR}^{k} - Z_{CTD}^{k})^{2}}{K}},$$
 (10)

In the RMSE calculation, the temperature of the corrected profile is linearly interpolated to the depth of the original error-free profile. The RMSE is used to represent the goodness of fit between the CTD and the corrected XBT profile at each set of locations. The minimum RMSE value provides the optimal locations of the switches. In the case of generating repeated locations,
we take the median value of the RMSE and derived error parameters to represent these locations.

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b) The maximum likelihood method for shipboard co-located data

The RMSE method described in (a) requires relatively expensive computation, neglects residual auto-correlation, and does not consider the error parameters simultaneously. Here we introduce a global optimization method to estimate simultaneously the mismatches between XBT/CTD colocated data (Section 2b). The optimization is performed using the dynamical evolution method (Storn and Price, 1997), an efficient method for sampling possible values of a parameter space θ and accounts for multimodality. This statistical model assumes that the temperature differences between the CTD and XBT observations are randomly distributed and auto-correlated.

According to equations (2b) and (3b), the temperature residual error is a random variable drawnfrom a multivariate normal distribution

 $E_T \sim N(T_0, \Sigma), \tag{11}$

with an unknown mean temperature or offset term T_0 , and a covariance matrix Σ , approximated by the residual variance σ_T^2 multiplied by an auto-correlation that decays exponentially between two depths Z_j and Z_k with a length scale λ :

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$$\Sigma_{jk} = \sigma_T^2 \exp(-|Z_j - Z_k| / \lambda) . \qquad (12)$$

We estimate simultaneously up to nine parameters $\theta = (T_0, z_0, z_d, z_2, \lambda, \sigma_T, Z(P_1), Z(P_2), Z(P_3))$, which are the XBT errors plus the optimal depths of the pressure switches. Out of these nine estimated parameters, six are estimated simultaneously. z_0 , z_d and z_2 are estimated separately, since they are derivative parameters calculated during the correction. The optimal values of these parameters are calculated by maximizing a Gaussian likelihood objective function $L(T \mid \theta)$ given for the temperature data conditional on the error parameters θ :

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$$L(T \mid \theta) \propto \exp\left(-\frac{(\Delta T^T \Sigma^{-1} \Delta T)}{2}\right), \qquad (13)$$

where $\Delta T = (T_{XBT} - T_0) - T_{CTD}$ is the residual temperature, which accounts explicitly for the temperature bias term T₀, and T_{XBT} is defined at the corrected depth Z_{CORR}, linearly interpolated to Z_{CTD}.

284

285 **4. Results**

We test the effectiveness of the pressure switch correction of simulated XBT profiles in three idealized experiments, using as base different climatological temperature profiles and sets of errors. As a first test, we validate the method to assure that it is capable of estimating the XBT error parameters

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291 **4.1 Simulated profiles**

292 To assess whether our approach is an unbiased estimator of the error parameters of an XBT

293 profile, we perform a simple experiment using a simulated profile. For an unbiased estimator, the

mean of the sampling distribution of one estimated parameter must be equal to the true value of

the parameter. In this experiment, the simulated XBT profile contains all typical errors (Table 1),

and the steps described in Section 3.2 are followed in order to estimate the error parameters.

297 Thus a linear version the correction approach is applied for $n \le 2$, and a quadratic version for $n \ge 2$

298 3. The residual errors (XBT minus CTD) are estimated using information from one to five

299 switches placed along the XBT temperature profile. A comparison between the error histograms estimated from the 12,500 realizations of the corrections using n = 1 to n = 5 pressure switches 300 and the original input errors used to simulate the XBT profile are shown in Figure 3. The largest 301 discrepancies are observed for the error estimates using only one switch (n = 1). In particular the 302 depth offset is poorly resolved, showing median values of -0.4 m, instead of the input value of z_0 303 304 = 5 m. The histograms of z_d and T_0 exhibit a long tail, showing that in this case the determination of the depth errors is subject to high uncertainty. For n = 2, T₀ and z₀ are precisely estimated, and 305 z_d is within the 60th percentile, but the median is located slightly above the correct value of $z_d =$ 306 3.6 m, to compensate for the missing quadratic term. For $n \ge 3$, there is a good agreement 307 between the input and estimated errors in most of the realizations of pressure switch locations, 308 309 confirming that this methodology is a potentially unbiased estimator of the FRE errors. As we increase the number of switches, the peak of the parameters histogram is slightly sharpened, 310 showing that in the case of a very dense number of switches the method reproduces the actual 311 312 temperature profile almost perfectly.

313

314 4.1.1 Number of pressure switches

Next, we explore the sensitivity of the correction of the XBT depth estimate using pressure switches to different errors and different numbers of pressure switches. We simulate three XBT deployments, each of them subject to different sets of measurement errors. To illustrate how the depth errors affect different profiles, we use as base three WOA09 climatological profiles from a tropical region, which have the strongest gradients. Different outcomes will be produced by the correction, thus each case (named a, b and c) will be analyzed separately as itemized below.

321 a) $(z_d, \varepsilon_z, \varepsilon_T, \varepsilon_p)$: In this experiment we apply only a linear depth bias and random errors into a tropical profile (Figure 4a). The median temperature residuals with respect to the CTD profile 322 323 (Figure 4b) show an improvement achieved by the depth correction independent of the number of switches. The original XBT profile shows higher deviation from the CTD profile in the 324 thermocline $\Delta T = 0.4^{\circ}$ C, where gradients are stronger. After the correction, temperature residuals 325 are mostly negligible, centered at $\Delta T = 0^{\circ}C$ along the whole profile. This is because the linear 326 depth biases, which cause an error of ~ 20 m at 700 m depth, are the only cause of temperature 327 328 errors in this simulated XBT profile, and these errors are efficiently reduced by a correction by 329 any number of switches (Figure 4c). The depth RMSE of the corrected profiles is sensitive to the location of the switches (Figure 4d, e), mostly because of the applied random errors. Random 330 errors affect the correction if the switches are placed relatively near each other, and the RMSE 331 decreases for a deeper location of the deeper switches (Figure 4d). The median RMSE of the 332 12,500 realizations show low variability among the number of switches applied in the correction, 333 ranging from 10^{-1} m < RMSE < 1 m, in comparison to RMSE ≈ 10 m for the uncorrected (n=0) 334 XBT depth (Figure 4e). Therefore, the correction provides a great improvement in the RMSE for 335 this set of errors towards the uncorrected XBT profile using any number of switches. The 336 thickness of the box plots in Figure 4e provides information about the variance of the correction, 337 and serves as an indicator for the optimal number of pressure switches. The more switches added 338 339 in this linear approach reduces the variance of the correction by averaging the random errors.

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b) $(z_0, z_d, \varepsilon_z, \varepsilon_T, \varepsilon_p)$: Here we add to the previous set of errors a depth offset (z_0) to the simulated XBT profile (Figure 5a). Increased temperature errors of up to 1.3°C are observed along the thermocline around 100 m depth (Figure 5b). After correcting the XBT profile with one pressure

switch (Figure 5b), there is still a noticeable residual temperature error of about 0.3° C in the 344 thermocline. Indeed, the addition of the depth offset z_0 mostly affects the correction using one 345 346 pressure switch. A residual linear depth bias remains after the correction using one switch (Figure 5c), with the linear form $E_z = 0.011*Z + 5.05$ m, which shows that z_d was reduced from 347 3% to ~1%, but $z_0 \approx 5$ m is still present in the corrected profile. Best results for one switch are 348 349 achieved if the switch is located deeper in the water column, below 400 m (Figure 5d). In comparison to the integral error of the uncorrected XBT profile (RMSE = 17 m; Figure 5e), the 350 351 correction with two or more switches in this linear approach can efficiently eliminate most this 352 bias, reducing the error to a RMSE = 0.1 m. Inaccurate information about the surface pressure can bring very different outcomes to the one switch correction (Figure 5e), shown by the 353 increased variance of this correction with respect to the experiment (a). This feature illustrates 354 that the depth bias offset (Z_0) can have an important role in producing residual linear depth 355 biases after the correction with one switch. 356

c) (T₀, z₀, z_d, z₂, ε_z , ε_T , ε_p): In this experiment we use an additional quadratic term (z₂) in the FRE 357 bias, as described in equation (8). For this $z_2 = 1e^{-5} m^{-1}$, which agrees with recent estimates 358 (Hamon et al., 2011). This bias term represents an acceleration term, which appears in some 359 360 XBT measurements caused by the probe adjustment to the terminal velocity (Cowley et al., 361 2012). We use this experiment to contrast the linear versus the quadratic fit of the equation (5), in the presence of a quadratic depth error. The linear fit is used for the correction with one and 362 two switches, and the quadratic fit is used for three or more switches, because more than three 363 364 switches support the degrees of freedom necessary for the quadratic regression. We explore the 365 results using a tropical profile (Figure 6a).

In this experiment we also add a temperature offset T_0 and analyze how T_0 can be detected after the depth correction. Results from this experiment show that one switch cannot detect the temperature offset well (Figure 6b), since there are still strong depth errors associated to the corrected profiles. Surprisingly, two switches are able to detect reasonably well the thermal offset of $T_0 = 0.2$ °C after the correction (Figure 6b), a result similar to the correction with three switches.

Three or more switches can reduce the depth biases to nearly zero in the whole water column 372 373 (Figure 6c). However, because the quadratic fit has more degrees of freedom, three switches show a high variance in comparison to the two switches case (Figure 6e). More than four 374 switches can restrict the variance of the quadratic fit given the simulated measurement errors. 375 The linear fit used for two switches can also constrain the depth bias in most of the profile 376 (Figure 6c). In the bottom of the profile errors are on order of 2 m, but the median of the residual 377 378 error (RMSE < 1m) is similar to the RMSE after the quadratic correction using three switches (Figure 6e), showing that a linear approach can still reasonably correct profiles with typical 379 acceleration biases of $z_2 \approx 1e^{-5} \text{ m}^{-1}$. Additional simulations (not shown) with increased 380 acceleration bias $(z_2 > 1e^{-4} m^{-1})$ show that the linear fit cannot constrain these errors, and the 381 RMSE increases to about 10 m. 382

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384 *4.1.2 Errors in the pressure measurement*

The accuracy of the depth correction is dependent on the accuracy of the pressure switch measurements. The accuracy of the pressure switches is greatly dependent on the quality of the equipment. Manufacturing costs of the pressure switches have to be considered when producing

such equipment to achieve the best performance at the lowest possible cost. Therefore, it is crucial to assess how errors in pressure switch measurements can affect the accuracy of the correction, and what is their acceptable range.

Current technology is available to make this task relatively easy and inexpensive. This technology will allow including discrete pressure measurements with accuracy of 0.85 m to 1 m (Sippican, personal contact). Therefore we use $p_0 = 1$ m as a threshold for the pressure switch accuracy in the present experiment, and estimate the depth RMSE after the correction with *n* switches.

Following the same methodology of the previous subsection, we use a simulated profile with typical XBT errors (Table 1), draw 12,500 random realizations of the location of the pressure switches, and analyze the residual biases after correcting the profile with these measurements. In addition to the precision errors, which are approximated by Gaussian random errors $\varepsilon_p = N(0, \sigma_p^2)$ with $\sigma_p = 0.1$ m in equation (4), we include a pressure offset term (p₀) varying between 0 and 5 m in 0.2 m increments. Equation 4 therefore becomes:

$$P = P_{CTD} + p_0 + \varepsilon_p \,. \tag{14}$$

The median of the distribution of the RMSE of the 12,500 realizations as a function of the random errors and number of pressure switches is shown in Figure 7. For small pressure errors $(p_0 < 2 \text{ m})$, there is a large gain of accuracy in going from one switch to two switches, but not much improvement is gained when more pressure switches are added. At higher pressure errors, the corrections with one and two switches show similar RMSE, when $p_0 \approx z_0$, since z_0 is the error inherent to the surface measurement using one switch correction. Accuracy is improved by adding more than two switches, which averages the random errors, as well as by using a 410 quadratic correction instead of a linear, which improves the RMSE on the order of 0.5 m to 1 m 411 for errors deep in the profile. Using $p_0 = 1$ m as a threshold, the RMSE = 1.6 m for two switches 412 and RMSE = 1 m for three or more switches. One pressure switch gives an RMSE > 3 m for the 413 considered threshold.

414

415 **4.2 Correction of actual co-located CTD/XBT data**

416 Here we test the ability of our approach in correcting XBT measurements biases using 417 simultaneous CTD and XBT deployments. Results shown here are from 19 collocated CTD and XBT casts collected in the tropical Atlantic. This data have previously been analyzed by DiNezio 418 and Goni (2011), which used the temperature gradient method to correct the XBT depth errors, 419 420 and diagnosed the average errors among these profiles of $z_d = 3.77 \pm 0.57$ % of depth, $z_0 = 0.2 \pm$ 421 1.54 m, and $T_0 = -0.03 \pm 0.17$ °C. We compare our results with those from DiNezio and Goni (2011) as a validation for the present method. A comparison of the XBT profiles from other 422 423 manufacturing years was also performed on this dataset, but not shown here, since it produced 424 similar results. The profiles are smoothed with an 11 m triangular window to avoid spikes and 425 interpolated to a 10 m vertical resolution. In this dataset, the XBT and the CTD data are available on the same vertical grid. Therefore, to simulate the pressure switch measurements, we 426 427 interpolate the CTD data to the corrected XBT depth estimated by DiNezio and Goni (2011) using the temperature gradient method. This step generates undesirable noise, inherent from the 428 429 gradient method, but is necessary to construct the pseudo-pressure observations. The original XBT profiles (gray dots in Figure 8) show a cold bias with respect to the CTD 430 profiles, evident as a median displacement to the left of about 0.2 °C in the temperature residuals 431

(Figure 8a, c, e). This is a joint effect of depth biases and thermal offset. In the thermocline, 432 located around 70-80 m, the cold bias intensifies (< -1°C in some profiles), a feature that is also 433 observed in the simulated profiles (Figures 4, 5 and 6). Depth differences of the original XBT 434 profiles relative to the CTD profiles show linearly increasing biases at depths below 150 m 435 (Figure 8 b, d, f), and are higher than 20 m at 700 m deep. Some outliers in the depth residuals 436 arise because we use the temperature gradient method of DiNezio and Goni (2011) to estimate 437 the CTD depths, as described in the beginning of this section, which is used to simulate the 438 439 pressure switch measurements.

We apply the pressure switch correction using one, two and three switches, using the quadratic 440 approach for three switches. The temperature biases after the correction are small, and most of 441 the temperature biases in the original XBT profile are result of depth errors, therefore the 442 443 temperature residuals after correction are mostly within the manufacturer's 0.2°C tolerance (colored dots in Figure 8a, c, e). Only in the correction with one pressure switch (Figure 8a) do 444 considerable mismatches still remain within the thermocline, with a maximum up to 1°C. For 445 two and three switches this maximum reduces to less than $\sim 0.5^{\circ}$ C. The depth biases after 446 correction (Figure 8b, d, f) are also mostly contained within the manufacturer's limits, but the 447 correction with one switch shows a much larger spread of the residuals than for two and three 448 449 switches.

450 The statistical optimization (Section 3.3b) estimates simultaneously, and for each cast

451 individually, the XBT measurement error and the optimal position of the switches to correct the

452 depth errors. The distributions of these optimal parameters are shown in Figure 9, and

453 summarized in Table 2 for the correction with one, two and three switches. The three corrections

are capable of reducing the RMSE considerably from the uncorrected XBT (Figure 9f). The
results show a median RMSE of ~3 m for the correction with one switch, and ~2 m for two and
three switches, against 14 m in the uncorrected XBT.

There is a wide range of possible optimal locations of the pressure switches (Figure 9e), and 457 particularly high variance is observed in the location for one pressure switch and for the deeper 458 switch in the two switches correction. Since the distributions of the estimated values parameter 459 460 are skewed (Figure 9), we use a bootstrap approach with 2000 samples to estimate the median and the standard deviation of the optimal depths of pressure switches. For one pressure switch 461 the optimal position is at mid-depth, $Z(P_2) = 289 \pm 198$ m. For two switches the optimal 462 463 positions are $Z(P_1) = 76 \pm 78$ m and $Z(P_2) = 593 \pm 168$ m, i.e., within the lower thermocline and deeper in the profile. Comparing the estimates of the XBT error parameters with the ones from 464 DiNezio and Goni (2011), results show that all estimated parameters are within the previously 465 estimated uncertainty. However, the one-switch correction estimates a negative median depth 466 offset ($z_0 = -0.85$ m) in comparison to a positive value in the other two estimates ($z_0 = 0.20$ m). 467

468

469 5. Conclusions

In this study we present an approach for correcting XBT depth bias using a discrete number of
pressure switch measurements. This approach can serve as a benchmark for the application of
pressure switches to correct XBT temperature profiles. We test this approach on several
experiments using tropical temperature profiles, by correcting simulated temperature profiles
with known errors added, and also by correcting co-located XBT and CTD casts.

475 Results obtained here indicate that the efficiency of the XBT depth correction is generally sensitive to the number of pressure switches employed. Using only one pressure switch can 476 result in a high variance in the efficacy of the correction because the depth offset cannot be 477 estimated with one switch only. A good improvement towards reducing depth errors is achieved 478 if the depth offset is absent or small, and the best quality of the depth correction can be achieved 479 480 if the switch is triggered around 300 m or deeper. The two pressure switches strategy shows the best tradeoff between the reduction of the XBT depth biases and the number of switches. It 481 482 improves on the one switch strategy by producing a much reduced variance of outcomes with 483 respect to the location of the switches, and a comparable RMSE to the correction with three switches. This result holds when we include typical quadratic errors ($z_2 \approx 1e^{-5} \text{ m}^{-1}$), which departs 484 slightly from a linear case and produces a depth error of 5 m at 700m. Sensitivity tests show that 485 for higher quadratic errors ($z_2 > 1e^{-4} m^{-1}$), applying two pressure switches becomes are less 486 efficient, producing an RMSE > 10 m. With three pressure switches, the correction improves 487 488 slightly from the two switches case by averaging random errors when a linear approach is applied. Three switches are able to detect the quadratic depth errors using a quadratic approach, 489 490 though their associated correction allows a high variance in a quadratic fit because of the low constraint for 2 degrees of freedom. Four or more switches can reduce random errors and 491 decrease the variance of a quadratic fit. Results from the collocated profiles in the tropical 492 Atlantic yield optimal switching positions at mid-depth of $Z(P1) = 289 \pm 198$ m for one switch, 493 and at the thermocline $Z(P1) = 76\pm78$ m and deep in the profile ($Z(P_2) = 593\pm168$ m) for two 494 switches. 495

By simulating variable accuracy in the pressure measurements, and accounting for typicalrandom errors, we use a threshold of 1 m for the pressure switch accuracy to infer the typical

498 RMSE for the correction of quadratic depth errors. The correction using one pressure switch 499 results in an RMSE > 3.5 m, for two switches an RMSE = 1.6 m, and for three or more switches 500 an RMSE = 1 m.

According to the results shown here, the inclusion of pressure switches in XBT probes can be 501 beneficial for scientific purposes, especially in climate studies, by reducing uncertainties in 502 ocean heat content and sea level variability estimates. We expect our theoretical results to be 503 504 validated in the tropical regions with real pressure switch measurements to be included in XBT 505 prototype probes. Regional characteristics include changes in environmental properties of the water, such as kinematic viscosity, which is highly dependent on the temperature (Seaver and 506 507 Kuleshov, 1982). Errors should vary geographically, following the local water temperature (Green, 1984; Hanawa, 1995; Thadathil et al., 2002), and the position of the switches could 508 possibly vary too. We do not explicitly account for the latitudinal variability of errors. 509 510 Additional improvements on the XBT probe or comparisons with other temperature profiles are required to correct pure thermal biases. A thermal offset (typically $T_0 \approx 10^{-1}$ °C) may be caused, 511 for example, by the recording system (e.g. Cowley et al., 2012), and the accuracy of the 512 513 temperature measurement in comparison to a static calibration of the thermistor is limited by the high falling speed of XBT probes (at least, six times faster than the CTD). Comparing the depth 514 corrected XBT with CTD profiles, or using an XBT tester probe (with fixed and well known 515 516 resistances), for example, can provide quantification of the XBT thermal offset of the whole 517 XBT system (probe + cable + recording system). New probes with improved thermistors and calibrations will aid to reduce temperature biases that would still remain after the depth biases 518 519 correction.

520

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Figure 1: Upper panel: Global upper ocean (0-700 m) heat content anomaly (OHCA) as a function of angle (in radians) for one cycle of simulated sinusoidal depth linear biases with amplitude of 2% of depth, based on the WOA09 annual climatology dataset. Lower panels: respective depth bias (Δz) located at the each circle of the angle space in the upper panel. In this illustration, OHCA is the average of 30 realizations which 50% of the world ocean temperature profiles are randomly selected to include the depth biases, therefore simulating the percentage of XBT observations in the World Ocean Database (WOD) during 1967-2001.

Figure 2: Schematic of the pressure switch correction. During the descent of the probe (probe not to scale), a temperature profile is produced. Pressure switches installed in the probe are triggered at various depths, and the recorded measurements P_1 , P_2 , ..., P_n correct the profile to the CTD depth.

Figure 3: Histogram of the error parameters (a) T_0 , (b) z_d and (c) z_0 , reproduced after correction of one XBT profile. Colored lines represent the corrections with different number of pressure switches applied, n = 1, 2, 3, 4 and 5 respectively. The gray dashed lines are the input errors introduced in the simulated XBT profile that are being estimated.

Figure 4: a) Temperature profiles for CTD (blue circles), XBT (green line with crosses), and corrected XBT profiles that minimize the RMSE using one (n=1; black line), two (n=2; red line), and three (n=3; cyan line) switches. b) Temperature and c) depth differences from the CTD for the XBT (green), n=1 (black), n=2 (red), and n=3 (cyan); d) Median RMSE (m) of the clustered 12,500 random realizations as a function of the depth of the deepest switch for n=1 (black), n=2 (red), and n=3 (cyan); and e) box-whisker plots showing the 0, 5, 25, 50, 75, 95 and 100 percentiles of RMSE (m) distribution for all 12,500 realizations for the XBT (n=0) and n=1 to 5 pressure switches. The XBT profile is simulated using the parameters (z_d , ε_T , ε_Z , ε_p).

- **Figure 5:** Same as Figure 4 but for errors $(z_0, z_d, \varepsilon_T, \varepsilon_Z, \varepsilon_p)$.
- **Figure 6:** Same as Figure 4 but for errors $(z_0, T_0, z_d, z_2, \varepsilon_T, \varepsilon_Z, \varepsilon_p)$.

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661 (c), and (e) are the temperature differences $(T_{xbt} - T_{ctd})$ in °C and (b), (d), and (f) are depth

differences in meters. Gray dots are for the original XBT profiles and colored dots for the

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dashed black lines represent the confidence intervals given by Sippican (0.2°C for temperature

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Figure 9: Box-whisker plots showing the 5,25,50,75 and 95 percentiles of the error parameter

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672 Figures:



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Parameter	Symbol	Typical values
Thermal offset	T_0	0.2 °C
Depth offset	Z ₀	5 m
Linear depth bias	Zd	3% of depth
Quadratic depth bias	Z ₂	$1e^{-5} m^{-1}$
Depth precision	ε _Z	0.001 m
Temperature precision	ε _T	0.01 °C
Pressure measurement error	ε _p	0.1 dbar (or m)

Table 1: Error parameter values in the XBT measurements used in this study.

Table 2: Bootstrapped median and standard deviation of the parameters values optimized for the 19 collocated CTD/XBT profiles, summarizing the results in Figure 9. The parameters are listed in the first column. The second to fourth columns are for the correction using one, two and three pressure switches. The fifth column shows the medians and standard deviations of the parameter values estimated by Dinezio and Goni, 2011 (DG11), when estimates are available.

764

n	1	2	3	DG11
σ _T (°C)	0.08±0.07	0.06±0.07	0.05±0.07	
Τ ₀ (°C)	-0.001±0.166	-0.01±0.15	-0.04±0.15	-0.03±0.17
z ₀ (m)	-0.82±1.79	0.20±1.21	0.22±1.5	0.20±1.54
z _d (%)	-3.48±1.1	-3.96±0.66	3.67±2.3	-3.77±0.57
$z_2 (m^{-1})$			$-0.49e^{-5} \pm 4.3e^{-5}$	
Z (P ₁) (m)	0	76±78	69±31	
Z (P ₂) (m)	289±198	593±168	320±113	
$\overline{\mathbf{Z}(\mathbf{P}_3)}(\mathbf{m})$			542±87	
RMSE	3.1 ± 4.3	1.9±1.3	2.1±2.3	