A potential bias in coral reconstruction of sea surface temperature

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[1] Isotopic measurements in corals are used to reconstruct past sea surface temperature. These reconstructions are based on calibration regression analyses using paired measurements of modern isotopic composition and sea surface temperature. It is shown that error in these measurements of sea surface temperature can lead to substantial bias in reconstruction. Provided the variance of the measurement error is known or can be estimated, a simple correction can eliminate this bias. *INDEX TERMS:* 0910 Exploration Geophysics: Data processing; 1050 Geochemistry: Marine geochemistry (4835, 4850); 4267 Oceanography: General: Paleoceanography. **Citation:** Solow, A. R., and A. Huppert (2004), A potential bias in coral reconstruction of sea surface temperature, *Geophys. Res. Lett.*, *31*, L06308, doi:10.1029/2003GL019349.

1. Introduction

[2] Isotopic and other geochemical measurements in corals have been used to reconstruct past sea surface temperature [*Beck et al.*, 1992; *Fairbanks et al.*, 1997; *Gagan et al.*, 2000]. As reviewed in more detail below, reconstruction is based on a model of the relationship between the isotopic measurement and sea surface temperature. The model is fit by regression using a calibration sample consisting of paired isotopic and sea surface temperature measurements. This fitting assumes that sea surface temperature is measured without error during the calibration period. This assumption is not always realistic. For example, error can arise when sea surface temperature is not measured at the location of the coral or when the pairing of sea surface temperature and isotopic measurements is imperfect. The purpose of this paper is to analyze the effect of a violation of this assumption on reconstruction. The analysis shows that measurement error can lead to a substantial bias in reconstruction. Provided a good estimate of the variance of the measurement error is available, this bias can be essentially eliminated by a simple correction.

2. The Effect of Measurement Error on Reconstruction and Its Correction

[3] Let Y denote an isotopic measurement in a coral and let SST denote the corresponding sea surface temperature. These quantities are assumed to be related through the simple linear regression model:

$$Y = \beta_o + \beta_1 SST + \varepsilon \tag{1}$$

where β_o and β_1 are unknown regression parameters and ε is an error with mean 0 and unknown variance σ_ε^2. This error includes both error in the isotopic measurement and variability in Y unrelated to variability in SST. This model can be fit by ordinary least squares (OLS) regression using a calibration sample consisting of paired isotopic and SST measurements. Let $\hat{\beta}_o$ and $\hat{\beta}_1$ be the estimates of β_o and β_1, respectively.

[4] Suppose now that an isotopic measurement Y_o is made outside the calibration sample. Interest centers on reconstructing the corresponding sea surface temperature SST_o. The reconstructed value found by inverting equation (1) is:

$$\hat{SST}_o = (Y_o - \hat{\beta}_o)/\hat{\beta}_1 \tag{2}$$

Provided that the estimates $\hat{\beta}_o$ and $\hat{\beta}_1$ are unbiased and that SST_o is not too far outside the SST range in the calibration sample, $\hat{SST}_o$ is also approximately unbiased. The alternative approach based on interchanging Y and SST in the regression equation is known to perform worse, particularly in extrapolating to conditions outside the calibration sample [e.g., *Shukla*, 1972].

[5] Returning to the calibration regression, suppose that, in addition to measurement error in Y, there is measurement error in SST. Specifically, suppose that:

$$SST_{meas} = SST_{true} + \eta \tag{3}$$

where SST_{meas} is measured sea surface temperature, SST_{true} is the true sea surface temperature, and η is a measurement error with mean 0 and variance σ_η^2. It is perhaps underappreciated that, in this case, the estimates $\hat{\beta}_o$ and $\hat{\beta}_1$ are biased [e.g., *Fuller*, 1987]. In qualitative terms, the effect of measurement error in SST is to attenuate the fitted regression model (i.e., on average, $\hat{\beta}_1$ is closer to 0 than β_1). This leads to what might be called accentuation in SST reconstruction, with the reconstruction of a cold SST being too cold and the reconstruction of a warm SST being too warm.

[6] It is possible to go beyond this qualitative result. Let σ_{SST}^2 be the variance of the values of SST_{true} in the calibration sample and let:

$$\lambda = \sigma_{SST}^2 / \left(\sigma_{SST}^2 + \sigma_\eta^2\right) \tag{4}$$

be the ratio of the variances of the true and measured values of SST in the calibration sample. It is well-known that, on average:

$$\begin{aligned} \hat{\beta}_1 &= \lambda\beta_1 \\ \hat{\beta}_o &= \beta_o + (1-\lambda)\beta_1\overline{SST} \end{aligned} \tag{5}$$

where $\overline{SST}$ is the mean of SST_{true} in the calibration sample [*Fuller*, 1987]. It follows upon substitution of these expressions into equation (2) that on average:

$$\hat{SST}_o = \frac{SST_o + (1-\lambda)\overline{SST}}{\lambda} \tag{6}$$

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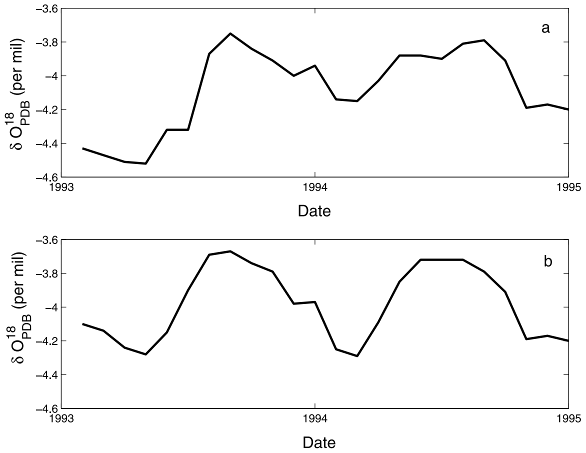

Figure 1. Time series of calibration $\delta^{18}O$ values for two Urvina Bay corals (a) Ur-1 and (b) Ur-3.

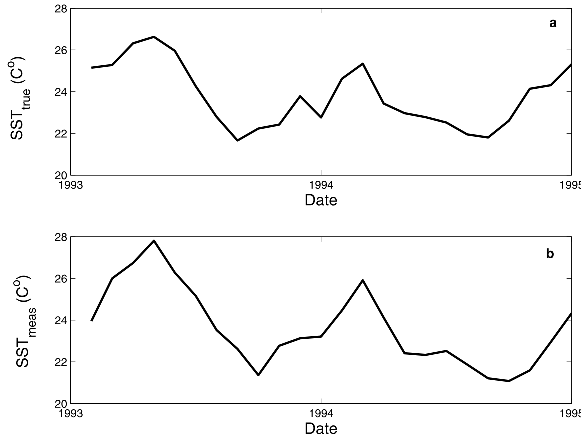

Figure 2. Time series of calibration *SST* values for (a) Urvina Bay and (b) Bartolomé.

Finally, upon substituting the expression for λ in equation (5) into equation (6) and subtracting the result from the expression for SST_o, the average reconstruction bias is:

$$SST_o - \hat{SST}_o \cong \left(\overline{SST} - SST_o\right)\frac{\sigma_\eta^2}{\sigma_{SST}^2} \tag{7}$$

Provided that σ_η^2 is known or can be estimated, an estimate λ is given by:

$$\hat{\lambda} = \frac{\sigma_{meas}^2 - \sigma_\eta^2}{\sigma_{meas}^2} \tag{8}$$

where σ_{meas}^2 is the sample variance of the measured *SST* values in the calibration sample. This estimate of λ can be used to construct the bias-corrected estimates of β_1 and β_o:

$$\begin{aligned} \tilde{\beta}_1 &= \hat{\beta}_1/\hat{\lambda} \\ \tilde{\beta}_o &= \bar{Y} - \tilde{\beta}_1\overline{SST}_{meas} \end{aligned} \tag{9}$$

where $\bar{Y}$ and $\overline{SST}_{meas}$ are the average of the isotopic and *SST* measurements in the calibration sample, respectively. Finally, these estimates can be used in turn to construct an approximately unbiased reconstruction:

$$\tilde{SST} = \left(Y_o - \tilde{\beta}_o\right)/\tilde{\beta}_1 \tag{10}$$

3. An Illustration

[7] In this section, we illustrate the reconstruction bias and its correction discussed in the previous section using part of the Galapagos coral stable oxygen calibration data set of *Wellington et al.* [1996]. These data, which are described in detail in the auxiliary material by *Wellington et al.* [1996] and are available at http://www.ngdc.noaa.gov/paleo/coral/galapagos.html, consist of 24 monthly measurements of $\delta^{18}O$ (PDB) covering the period 1993–1994 extracted from each of two corals (designated as Ur-1 and Ur-3) of the species *Pavona clavus* at approximately 3 m depth in Urvina Bay, Isabela Island (0.23 S 91.14 W) in the Galapagos Islands, Ecuador.

[8] The two time series of $\delta^{18}O$ are plotted in Figure 1. Figure 2 shows the corresponding values of *SST* measured at the site. These measurements, which we will treat as correct (i.e., as SST_{true}), have average $\overline{SST}$ = 23.79°C and standard deviation σ_{SST} = 1.48°C. The estimates of the parameters β_o and β_1 found by OLS regression of $\delta^{18}O$ on SST_{true} for the two corals are given in Table 1.

[9] Suppose that the *SST* measurements at the Urvina Bay site had not been available and that measurements at another nearby site studied by *Wellington et al.* [1996] at Bartolomé are used instead in calibration (i.e., as SST_{meas}). The time series of SST_{meas} is also shown in Figure 2. The difference SST_{true} – SST_{meas} has average 0.15°C and standard deviation 0.92°C, which we will take as σ_η. The estimated value of λ is 0.72. The estimates of β_o and β_1 found by OLS regression of $\delta^{18}O$ in the Urvina Bay corals on SST_{meas} from Bartolomé are also reported in Table 1. These results are broadly consistent with the theoretical result in equation (5) - that, it should be emphasized, applies *on average* and not in each particular case. The bias-corrected estimates of β_o and β_1 given by equation (9) are also reported in Table 1.

[10] To illustrate the effects on *SST* reconstruction, Figure 3 shows *SST* reconstruction plots – that is, the reconstructed *SST* value as a function of the $\delta^{18}O$ measurement – for each of the two Urvina Bay corals based on the three sets of parameter estimates given in Table 1. The accentuation bias due to using SST_{meas} instead of SST_{true} in

Table 1. Estimates of β_o and β_1 for the Two Urvina Bay Corals Ur-1 and Ur-3 Based on Regressions of $\delta^{18}O$ on SST_{true} and on SST_{meas} and Based on Correcting the Latter for Bias According to Equation (7)

	Estimate of β_o	Estimate of β_1
Ur-1		
using SST_{true}	−0.44	−0.15
using SST_{meas}	−1.54	−0.11
bias-corrected	−0.49	−0.15
Ur-3		
using SST_{true}	−0.96	−0.13
using SST_{meas}	−2.13	−0.08
bias-corrected	−1.44	−0.11

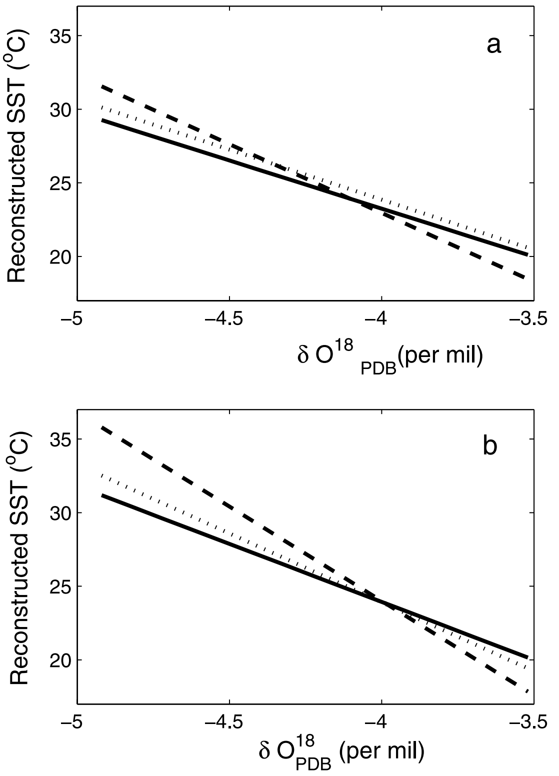

Figure 3. *SST* reconstruction plots for (a) Ur-1 and (b) Ur-3. In each case, the solid line is based on SST_{true}, the dashed line is based on SST_{meas}, and the dotted line is based on bias correction.

the calibration regressions is clear, reaching 1.5°C for $\delta^{18}O$ values within the range of the calibration data. The use of the bias-corrected estimates essentially eliminates this bias in the first coral and reduces it substantially in the second (e.g., a maximum reconstruction bias of 0.5°C for $\delta^{18}O$ values within the range of the calibration data).

4. Discussion

[11] The purpose of this paper has been to analyze the effect on *SST* reconstruction from corals of measurement error in calibration *SST* data. Although the paper has focused on reconstruction from isotopic measurements, the same results pertain to reconstructions from any proxy for which calibration is based on ordinary least squares. The basic result, given in equation (6), is that even relatively modest measurement error can lead to a relatively large accentuation bias, particularly at and beyond the range of conditions during the calibration period. Provided the variance σ_η^2 of the measurement error can be estimated, the bias-corrected reconstruction based on equations (8) and (9) provides a simple way to correct for this bias. The estimation of σ_η^2 , which is discussed below, is not always easy. However, even in the absence of a good estimate, the quantification of accentuation bias presented here can be useful for bracketing the potential reconstruction bias.

[12] Before proceeding, a word is in order about an alternative approach. A widely known approach to fitting a simple linear regression model in the presence of measurement error in the regressor is reduced major axis (RMA) or orthogonal regression. In OLS regression, the parameters are estimated by minimizing the sum of vertical deviations between the data points and the regression line. In contrast, in RMA regression, the parameters are estimated by minimizing the sum of orthogonal deviations between the data points and the regression line. *Shen and Dunbar* [1995] discussed this method in analyzing coral isotope records [see also *Quinn et al.*, 1998; *Quinn and Sampson*, 2002]. In terms of the model defined by equations (1) and (3), RMA regression assumes that the variance of ε is equal to the variance of η. There is no reason to believe that this assumption is warranted. The method can be extended to allow for differences in these variances [see, e.g., *Carroll et al.*, 1995]. To do so, it is necessary to have an estimate of both variances. As ε includes both isotopic measurement error and natural variability in Y unrelated to *SST*, it is not sufficient to consider only the variance of the former in this extension. More generally, finding a good estimate of the variance of ε is not straightforward. In particular, the estimate based on OLS regression will be biased in the presence of measurement error in *SST* [*Carroll et al.*, 1995]. A final disadvantage is that, even with estimates of the variances of ε and η, the actual fitting can be complicated.

[13] Returning to the method described in this paper, the estimation of σ_η^2 depends on the specific nature of the measurement error. When the time series of SST_{true} is short or absent altogether, one common approach is to use a spatial interpolation or gridding algorithm to estimate SST_{true} from measurements at a number of one or more nearby locations. When this is done to *extend* the calibration period beyond that covered by the time series of SST_{true}, then the period of overlap may be long enough to allow estimation of σ_η^2. When this period of overlap is very short or non-existent, then estimation of σ_η^2 must be based on a knowledge of spatial variability in *SST* as reflected, for example, in the spatial covariance function [*Kaplan et al.*, 1998]. In fact, many gridding methods provide a direct estimate of the variance of the interpolation error which corresponds to σ_η^2. It is worth pointing out that the use of a poor estimate of σ_η^2 could lead to a bias-corrected reconstruction whose bias is actually greater than that of the uncorrected reconstruction.

[14] Finally, it has been assumed in this paper that the goal is to reconstruct SST_{true} (i.e., at the site of the coral). If instead the goal is to reconstruct SST_{meas}, then the issue of measurement does not arise. However, this does assume a linear relationship between SST_{true} and SST_{meas} and that this relationship remains stable over the period of reconstruction.

[15] **Acknowledgments.** The helpful comments of four anonymous reviewers are acknowledged with gratitude.

References

Beck, J. W., R. L. Edwards, E. Ito, F. W. Taylor, J. Recy, F. Rougerie, P. Joannot, and C. Henin (1992), Sea-surface temperature from coral skeletal strontium/calcium ratios, *Science*, *257*, 644–647.
Carroll, R. J., D. Ruppert, and L. A. Stefanski (1995), *Measurement Error in Nonlinear Models*, 305 pp., Chapman and Hall, New York.
Fairbanks, R. G., M. N. Evans, J. L. Rubenstone, R. A. Mortlock, K. Broad, M. D. Moore, and C. D. Charles (1997), Evaluating climate indices and their geochemical proxies measured in corals, *Coral Reefs*, *16*, 93–100.
Fuller, W. A. (1987), *Measurement Error Models*, 440 pp., John Wiley, Hoboken, N. J.
Gagan, M. K., L. K. Ayliffe, J. W. Beck, J. E. Cole, E. M. Druffel, R. B. Dunbar, and D. P. Schrag (2000), New views of tropical paleoclimates from corals, *Quat. Sci. Rev.*, *19*, 45–64.

Kaplan, A., M. A. Cane, Y. Kushnir, A. C. Clement, M. B. Blumenthal, and B. Rajagopalan (1998), Analyses of global sea surface temperature 1856–1991, *J. Geophys. Res.*, *103*, 18,567–18,589.
Quinn, T., and D. E. Sampson (2002), A multiproxy approach to reconstructing sea surface conditions using coral skeleton geochemistry, *Paleoceanography*, *17*(4), 1062, doi:10.1029/2000PA000528.
Quinn, T. M., T. J. Crowley, F. W. Taylor, C. Henin, P. Joannot, and Y. Join (1998), A multicentury stable isotope record from a New Caledonia coral: Interannual and decadal sea surface temperature variability in the southwest Pacific since 1657 A. D., *Paleoceanography*, *13*, 412–426.
Shen, G. T., and R. B. Dunbar (1995), Environmental controls on uranium in reef corals, *Geochim. Cosmichim. Acta*, *59*, 2009–2024.
Shukla, G. K. (1972), On the problem of calibration, *Technometrics*, *14*, 547–553.
Wellington, G. M., D. B. Dunbar, and G. Merlen (1996), Calibration of stable oxygen isotope signatures in Galapagos corals, *Paleoceanography*, *11*, 467–480.

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