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Sea Surface Temperature Reconstruction using 3D X-ray Computed Tomography in Coral Cores from Baler, Aurora, Philippines: An Initial Study

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Abstract

Massive coral species are essential archives of past sea surface temperature (SST) records as they incorporate biological and geochemical tracers that reflect temperature variations of their living marine environment. Existing methods of reconstructing past SST data involve analyzing elemental or isotopic ratios (e.g., Sr/Ca, coralline $\delta^{18}O$) that are known functions of seawater temperature. The potential of annual density bands of coral skeletons as an SST tracer has received less attention so far. 3D X-ray computed tomography (3DXCT) allows quick imaging of coral density bands with minimal to no sample preparation to extract relevant climate data as gray values (GV) – a measure of total X-ray absorption of the sample. Given the known influence of temperature on annual growth density bands and the GV profiles of corals, a novel method of SST reconstruction using GV from 3DXCT analysis, is presented. Two Porites spp. coral core samples (Baler 2 and 3) from Baler, Aurora, Philippines were analyzed using 3DXCT to obtain their GV profiles. GV profiles were matched with existing SST data (optimally interpolated SST). Comparisons showed significant positive linear correlation with equations SST = 0.3645 GV + 10.414 (r^2 = 0.6389) and SST = 0.462 GV – 1.8888 (r^2 = 0.7845) for Baler 2 and 3, respectively. SST reconstructed using these linear equations had mean absolute errors of 3.4 and 2.9% compared with OISST for Baler 2 and Baler 3, respectively. These findings showed the potential of 3DXCT analysis of coral cores as a relatively easy, quick non-destructive and precise method for SST reconstruction.

Keywords*:* 3DXCT, corals, gray value, Philippines, sea surface temperature

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1. Introduction

Sea surface temperature (SST) is one of the most studied parameters in oceanographic and paleoclimatic studies as it is linked to general oceanic, atmospheric and meteorological behavior (Ellis *et al.*, 2019). SST is also considered as one of the essential climate variables (ECVs) developed by the Global Climate Observing System (GCOS) program to aid climate monitoring, research, applications and policymaking (Bojinski *et al.*, 2014; Emery, 2015; Banzon *et al.*, 2016; Bautista *et al.*, 2021).

One of the most prominent SST datasets in climate studies is optimally interpolated SST (OISST). OISST refers to several data sets formed from combining in situ and satellite data to obtain a higher spatial and temporal resolution. For example, Reynolds *et al*. (2007) have developed an OISST data set with a spatial grid resolution of 0.25° and temporal resolution of one day. This particular daily OISST dataset is only available from September 1981 to the present (Banzon *et al.*, 2016). These limitations in the temporal coverage of available SST data hinder one's ability to gain information on past and current environmental systems and predict future rates of climate change (Cardinal *et al.*, 2001; Flannery *et al.*, 2016; Ramos *et al.*, 2017). Thus, reconstruction of SST records is essential for the advancement of paleoclimatic research.

Paleoclimatic studies often utilize geologic archives such as corals, ice cores and tree rings to retrieve climate data beyond the existing instrumental records (Quinn and Sampson, 2002; Tierney *et al.*, 2015). In particular, massive tropical corals have been greatly useful in SST reconstruction because they are widely distributed, their growth cycles are widely known, they live in shallow waters (< 50 m), they can be accurately dated, and they continue growing amidst the presence of environmental stressors (Correge, 2006; Lough and Cantin, 2014; D'Olivo *et al.*, 2018). Moreover, they incorporate different isotopic and geochemical tracers within their skeleton that vary based on various environmental factors such as SST when the skeleton was formed (Gagan *et al.*, 2000; Ellis *et al.*, 2019; Tao *et al.*, 2021). During the past decades, Sr/Ca is considered the most reliable tracer for SST reconstruction due to the established negative correlation of [Sr] to SST (Beck *et al.*, 1992; Cardinal *et al.*, 2001; Cahyarini *et al.*, 2009). Another standard tracer is coralline $\delta^{18}O$. However, it is less reliable than Sr/Ca ratios because coralline $\delta^{18}O$ is also controlled by local evaporation-precipitation equilibrium (Cardinal *et al.*, 2001). Less frequently, U/Ca and Mg/Ca ratios from coral skeletons have also been explored in paleo-reconstruction of SST data (Wei *et al*., 2000; Fallon *et al*., 2003; Patterson *et al*., 2021). However, these existing methods are expensive and time-consuming and involve extensive subsampling and wet chemistry techniques to obtain accurate and precise elemental data (Ellis *et al*., 2019). Another limitation of using trace element paleothermometers is the need for colony-specific temperature calibrations (D'Olivo *et al*., 2018).

In recent years, researchers explored the annual growth band characteristics (i.e., skeletal density, calcification and extension rates) of massive tropical corals and their potential as intrinsic chronometers of environmental information (Barnes and Lough, 1993; DeCarlo, 2017). These growth parameters are generally interrelated and highly connected to the coral's living marine environment (Baumann *et al*., 2019; Courtney *et al*., 2017). Early studies theorized that light and temperature are the principal environmental factors influencing the couplets of alternating high- and low-density bands of massive coral calibrations (D'Olivo *et al*., 2018). High-density bands are formed during high temperatures, while low-density bands are formed during low temperatures (Benson *et al*., 2019). Other possible factors include freshwater runoff, latitude, rainfall and sea level pressure, among others, although their impacts are still not fully understood (Highsmith, 1979; Dodge and Vaisnys, 1980; Barnes and Lough, 1996; Lough and Barnes, 2000; DeCarlo, 2017; Rawson *et al*., 2020). Although it is still not fully understood how coral density bands are formed, studies show that SST plays an essential role in its development (Sun *et al*., 2002).

Digital imaging of these coral density bands, which involves the analysis of color values in a digital image of a sample, has received less attention in paleoclimatic reconstruction studies so far. Sun *et al*. (2002) reviewed the potential of digital image analysis in extracting environmental signals from geological archives. It generally involves three main procedures: (1) image acquisition (usually through X-ray imaging), (2) image analysis and (3) correlation of acquired image data to governing environmental factors. One of the parameters in an X-ray image is the gray value (GV), a measure of the lightness or darkness of a data point. This value corresponds to the total X-ray absorption through the given sample, which is related to the density and thickness of the sample (Wang *et al*., 2010). Thus, for coral cores of a fixed thickness, parts with higher density should register higher gray values in a negative X-ray image and vice versa. Given this, GV provides a proxy index of coral skeletal density, which in turn can be used to reconstruct the living marine conditions of the coral samples.

Three-dimensional (3D) X-ray computed tomography (3DXCT) is a fast, non-destructive and non-invasive imaging technique used for the 3D visualization and characterization of an object of interest. It involves the capture of multiple X-ray projections from different angles around the sample. Dataset from the projections is digitally reconstructed, producing a grayscale 3D image that shows the variations of X-ray attenuation within the investigated sample (Laforsch *et al.*, 2008; Rawson *et al.*, 2020). These attenuations are related to density, which corresponds to the density variations and boundaries in the sample's internal structure (Ketcham and Carlson, 2001). Because minimal to no sample preparation is involved in 3DXCT, the sample remains available for further downstream analysis (Angeletti *et al.*, 2019). 3DXCT has a distinct edge over the more commonly used 2D X-ray techniques. The 3D imaging capabilities of 3DXCT produce a reconstructed 3D image of the whole coral core where one can freely choose an optimum growth axis to reveal a more accurate image of the coral growth bands (Cantin *et al.*, 2010; Chan *et al.*, 2017). Initially developed for medical diagnosis, 3DXCT have been then successfully used in the advancements of a variety of disciplines including archaeology, geology, life sciences, material science, paleontology, petrology and soil science (Ketcham and Carlson, 2001; Carlson *et al.*, 2003; Mees *et al.*, 2003; Laforsch *et al.*, 2008; Taina *et al.*, 2008; Mooney *et al.*, 2012; Cnudde and Boone, 2013; Garcea *et al.*, 2018; Urbaniec *et al.*, 2018; Rawson *et al.*, 2020). To date, only a few published studies have utilized 3DXCT in coral studies, and no other studies have used 3DXCT to visualize annual density bands for high-resolution SST reconstruction to the best of the authors' knowledge (Sun *et al.*, 2002).

This paper presents a novel method to reconstruct SST data using 3DXCT analysis of *Porites* spp. coral cores from Baler, Aurora, Philippines. In particular, 3DXCT was used to visualize the annual growth bands and obtain the gray value profiles of the coral core samples and hence, reconstruct SST. The reconstructed SST data from the 3DXCT analysis is presented in this study and compared to the existing grid-SST data from OISST of Reynolds *et al.* (2007) and Banzon *et al.* (2016). Given the current limitations of available SST datasets, and the fact that long-lived corals record SST changes throughout their lifetime as density variations in their skeletons, 3DXCT imaging can be used to visualize annual density bands of corals for high-resolution SST reconstruction. In this work, it was demonstrated that this method can create high-resolution SST datasets from coral cores that augment and improve the currently available datasets.

2. Methodology

2.1 Sampling Site

Baler is a third-class municipality located in Aurora Province, Philippines. Baler's coastline and bay directly face the Pacific Ocean with seawater primarily coming from the Kuroshio Current or the northward bifurcation of the North Equatorial Current. The degree of seawater input from the Kuroshio recirculation gyre and North Pacific mode waters depends on the season: the El Niño Southern Oscillation and the Pacific Decadal Oscillation. Baler experiences an average seasonal SST range of 26.4 °C in February to 29.8 °C in June (Figure 1b; Reynolds *et al*., 2007).

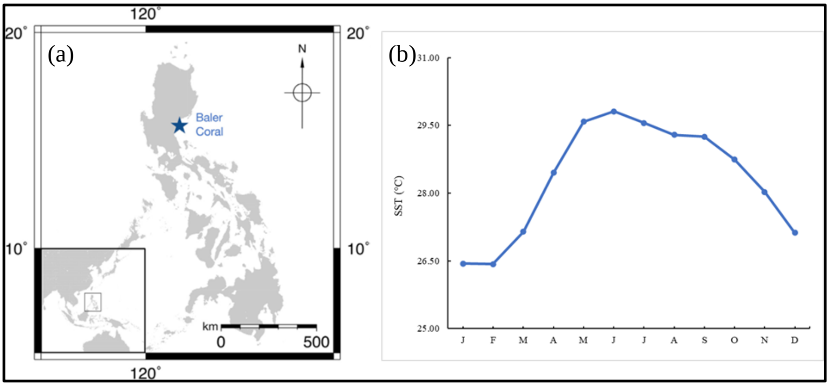

Figure 1. Coral sampling site in Baler, Aurora (a) and monthly mean SST of Baler Bay from 1982 to 2018 (b); data from OISST (Reynolds *et al*., 2007; Banzon *et al*., 2016)

2.2 Coral Sampling

The coral cores used in this study were from *Porites* spp., a massive tropical coral species common in Philippine waters. The sampling in Baler Bay (15.7587 °N, 121.6300 °E) was performed in October 2018, where two cores (referred to in this paper as Baler 2 and 3) were drilled from two different colonies of *Porites* spp. coral heads 5 m apart; both submerged about 5 m below sea level. Coral cores were obtained by drilling perpendicular to the coral growth using a diver-operated hydraulic drill apparatus. It was opted to drill one coral core per colony for this study to prevent too much damage to the colony. The lengths of Baler 2 and 3 coral cores were 82 and 89 cm, respectively. Baler 2 has a significant hole in its top segment likely caused by a burrowing marine organism. Thus, Baler 3 served as a duplicate coral core and provided the data for the damaged part of Baler 2. In this study, only the top 50- and 15-cm portions of Baler 2 and 3, respectively, were used as these correspond to the years with available daily SST records from OISST.

2.3 Sample Preparation and 3DXCT Analysis

The two coral cores were cut into 5-mm thick slabs using a customized circular saw cutter. The coral slabs from both coral cores were cleaned using ultrapure water and dried overnight at 40 °C in a clean oven. This cleaning step ensured samples were free of ocean residues and moisture. Slabs were subsequently wrapped and labeled appropriately. After washing and drying, the coral slabs were analyzed using 3DXCT (X5000, North Star Imaging, United States) with the following settings: 115 kV, 300µA, 34.5 focal spot size, microfocus focal spot mode at 12.5 fps. The radiographs of the coral slabs were cross-checked against each other for consistency; the slab at the middle of the coral core was then used for subsequent analysis.

From the resulting 3D image of the selected coral slab, a 2D image slice was obtained at 2.5 mm of the slab's thickness axis. Gray values (GV) from the resulting 2D image slice were determined per pixel from top to bottom of the coral slab with each pixel corresponding to a spatial resolution of 54 µm.

2.4 Data Repositories

Daily SST data (from February 1982 to sampling date) were obtained from the OISST; a 0.25° daily SST record constructed from the interpolation of multiple observations from various platforms (i.e., satellites, ships, buoys and Argo floats [Banzon *et al*., 2016]). Raw data of the coral GV and the age model or chronology construction of the Baler 2 and 3 coral cores have been previously accomplished and can be accessed in Bautista *et al*. (2021).

2.5 SST Reconstruction from Gray Values

X-radiographs of all coral core slabs were cross-checked against each other for consistency. The slab with the most precise details (e.g., minimal damage and artifacts), usually the slab at the middle of the coral core, was selected for SST reconstruction. The GV profile (i.e., peaks and troughs) across the length of the coral core were matched with the OISST time series profile in Baler using the QAnalysis software (Kotov and Pälike, 2018). As detailed in Bautista *et al*. (2021), this was also the basis of the coral age model or chronology, wherein QAnalySeries generated the age model for the Baler 2 and Baler 3 slabs after the matching step based on the age dates of the SST records. Each GV-SST match was called a "tie line." From all the tie lines, a linear equation was determined, and this resulting equation was used for the SST reconstruction of all other points on the time series. To determine the "goodness-of-fit" of the reconstructed SST, the temporal resolutions of OISST and the reconstructed SST were normalized by downscaling to monthly resolution. Subsequently, the mean absolute error (MAE or MAE%) of the reconstructed SST versus OISST is calculated using Equations 1 and 2.

$$MAE = \frac{1}{n}\Sigma \mid SST_{reconstructed} - SST_{OISST} \mid \tag{1}$$

$$MAE\% = \frac{\frac{1}{n}\Sigma \mid SST_{reconstructed} - SST_{OISST} \mid}{\frac{1}{n}\Sigma \mid SST_{OISST} \mid} \tag{2}$$

3. Results and Discussion

3.1 Matching Coral Gray Values and SST

3DXCT analysis of the Baler 2 coral core resulted in a total of 3,281 GV data points along the transect (straight red lines in Figure 2a) considering overlaps between the two coral slab segments. GVs ranged from 39.91 to 70.98 with an average of 59.63. The spatial resolution per data point (i.e., pixel) was 54 µm, which corresponded to a time resolution between one to 21 days, or an average of five days. On the other hand, 3DXCT analysis of the Baler 3 coral core resulted in a total of 993 GV data points along the transect (straight red line in Figure 2c). GVs ranged from 57.66 to 75.10 with an average of 65.81. The spatial resolution per data point (i.e., pixel) was 54 µm, which corresponded to a time resolution between one to 23 days, or an average of seven days.

Coral density is related to sea surface temperature (SST) fluctuations, wherein coral skeleton is formed with higher density during times of high SST and vice versa (Benson *et al*., 2019; Ellis *et al*., 2019). As such, in a negative 3DXCT image, high GV should denote high SST and vice versa. Based on this principle, the maxima and minima of the GV profile of Baler 2 and 3 were matched with SST data in Baler from OISST (Reynolds *et al*., 2007; Banzon *et al*., 2016). A total of 126 and 66 tie lines were identified for Baler 2 and Baler 3, respectively (Figures 2b and 2d).

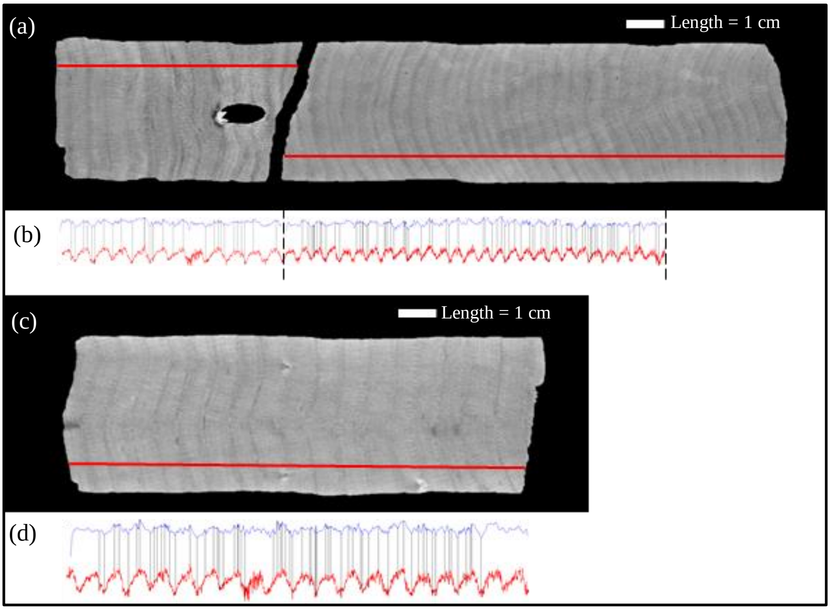

Figure has been modified from Bautista *et al.* (2021).

Figure 2. Annual density bands (L-R: from top to bottom of the coral slab) from 3DXCT images of Baler 2 (a) and Baler 3 (c) coral cores; straight red lines superimposed on the X-ray images corresponded to the area where gray values of the coral samples were taken. Gray value profiles (blue curve) of Baler 2 (b) and Baler 3 (d) matched with the SST profile in Baler, Aurora based on OISST (red curve).

Linear regression was performed between GV-SST tie lines showing significant positive correlations for both Baler 2 and Baler 3, which yielded linear equations of SST = 0.3645GV + 10.414 with r^2 = 0.6389 and SST = 0.462GV – 1.8888 with r^2 = 0.7845, respectively (Figure 3).

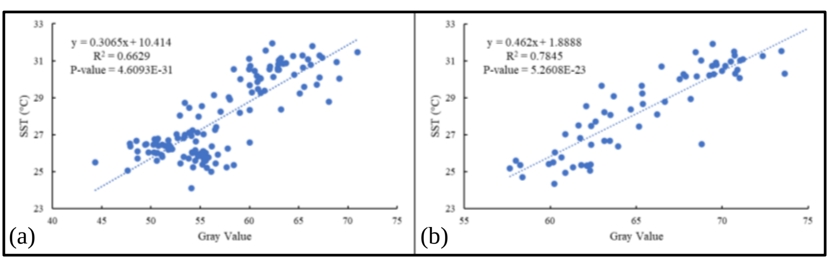

Figure 3. Plot of Baler 2 (*n* = 126) (a) and Baler 3 (*n* = 66) (b) coral gray values against instrumental SST data (i.e., OISST) of the Baler sampling site

This finding agrees with the established knowledge that high-density bands, denoted by high gray values, are produced during periods of high temperature and vice versa. Moreover, this finding indicates that 3DXCT GV of coral cores can be used to estimate and reconstruct SST, particularly important for older parts of the coral core when SST data is not yet existent.

However, it is notable that Baler 2 has a lower r^2 value, possibly because its two coral slab segments were analyzed separately, and their datasets were only combined after (the two slabs had different linear equations). Aside from coral density and thickness, GV would be affected by other factors such as 3DXCT measurement parameters and the position of the sample in the analysis chamber. Changes in these factors will affect the resulting GV, and in this respect, GV remains an arbitrary measure. In this study, it was endeavored to keep the other factors constant (i.e., slab thickness, 3DXCT measurement parameters and sample position). Nonetheless, in future studies, it is recommended that a density calibration standard with a similar matrix to the corals be made and used to anchor all measurements and eliminate fluctuations due to other factors aside from density variations in the coral core.

3.2 SST Reconstruction and Fitting

Using the GV-SST linear equations of the Baler 2 and 3 coral cores, the SST of each GV data point in both coral cores were calculated. The calculated SST data from OISST was then compared to determine the accuracy of SST reconstruction (Figure 4). To make a 1:1 comparison of all data points, the time resolution of both calculated SST and OISST datasets was normalized by scaling them down to monthly resolution (i.e., by taking the average monthly SST based on available data points). In particular, Baler 2 record is from September 1981 to September 2018, and the Baler 3 record is from February 2000 to June 2019. An additional correction value of -3.685 °C was used for Baler 2 to improve the reconstruction accuracy as there appeared to be positive bias when only the linear equation was used for the SST reconstruction. This may again be because the two coral slab segments of Baler 2 were analyzed separately resulting in some fluctuations in GV. No correction value was needed for Baler 3.

Furthermore, the reconstructed SST based on the GV profile of Baler 2 had a mean absolute error (MAE) of 0.96 °C (or a MAE% of 3.4%) compared with OISST. On the other hand, the reconstructed SST based on the GV profile of Baler 3 had an MAE of 0.86°C (or a MAE% of 2.93%) compared with OISST. Both reconstructed SST datasets followed similar sinusoidal seasonal temperature cycles showing annual warmer SSTs during June to August and cooler SSTs during January to March. Their time-series graphs (Figure 4) showed a precise visual match between reconstructed SST data and the OISST.

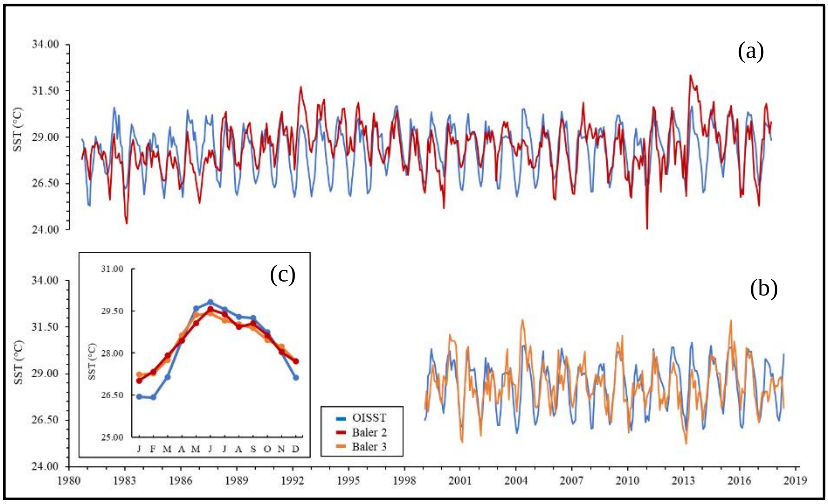

Figure 4. Monthly average reconstructed SST records from Baler 2 (red curve) (a) and Baler 3 (orange curve) (b) coral gray values overlain with SST records from OISST (blue curve); overall monthly average SST data of OISST, Baler 2, and Baler 3 from 1982 to 2018 (c)

4. Conclusion and Recommendation

This study showed the potential of 3DXCT analysis of coral cores for reconstructing SST. Gray values from Baler 2 and Baler 3 coral cores revealed significant positive correlations with OISST data. In particular, reconstructed SSTs based on SST versus GV linear equations yielded MAE% of 3.4 and 2.9% for Baler 2 and Baler 3, respectively. These results demonstrated the degree of accuracy of SST reconstruction based on 3DXCT GV with the current methodologies. It was indicated that 3DXCT GV has the potential to be a quick, easy and accurate tool for determining the age models of coral cores based on monthly to annual coral density and SST fluctuations, as well as reconstructing SST records of the past, particularly important for older parts of the coral core when SST data is not yet existent.

Furthermore, several recommendations are highlighted for future studies as a way forward for fully establishing this method for SST reconstruction. As gray values may vary depending on the nature and species of the coral sample, 3DXCT instrument used, its settings and specifications and the position of the sample in the analysis chamber, it is recommended to establish and use a coral density standard that can be used to calibrate and anchor future gray value measurements of coral cores. Moreover, the study was based on a single line GV out of multiple GV lines available. Thus, there is a need to explore the potential of using a multi-cross-sectional average of the GV for each band to come up with more robust data. The method also needs to be applied to a larger number of coral core samples from various locations and of different coral species and should be compared with other established proxies for SST reconstruction (e.g., Sr/Ca, coralline $\delta^{18}O$). Lastly, to comprehensively analyze the application of coral gray values as a marine paleothermometer and environmental proxy, other factors that may affect its variations should also be examined.

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