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Mg/Ca, Sr/Ca AND STABLE ISOTOPE FROM PLANKTONIC FORAMINIFERA *T. SACCULIFER*: TESTING A MULTI-PROXY APPROACH FOR INFERRING PALEO-TEMPERATURE AND PALEO-SALINITY

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ABSTRACT

Over the last decades, sea surface temperature (SST) reconstructions based on the Mg/Ca of foraminiferal calcite have frequently been used in combination with the $\delta^{18}O$ signal from the same material, to provide estimates of $\delta^{18}O$ of the water ($\delta^{18}O_w$), a proxy for global ice volume and sea surface salinity (SSS). However, because of error propagation from one step to the next, better calibrations are required to increase accuracy and robustness of existing isotope and element to temperature proxy-relationships. Towards that goal, we determined Mg/Ca, Sr/Ca and the oxygen isotopic composition of *Trilobatus sacculifer* (previously referenced as *Globigerinoides sacculifer*), collected from surface waters (0-10m), along a North-South transect in the eastern basin of the tropical/subtropical Atlantic Ocean. We established a new paleo-temperature calibration based on Mg/Ca, and on the combination of Mg/Ca and Sr/Ca. Subsequently, a sensitivity analysis was performed in which, one, two, or three different equations were considered. Results indicate that foraminiferal Mg/Ca allow for an accurate reconstruction of surface water temperature. Combining equations, $\delta^{18}Ow$ can be reconstructed with a precision of about ±0.5‰. However, the best possible salinity reconstruction based on locally calibrated equations, only allowed reconstruction with an uncertainty of ±2.49. This was confirmed by a Monte Carlo simulation, applied to test successive reconstructions in an 'ideal case', where explanatory variables are known. This simulation shows that from a pure statistical point of view, successive reconstructions involving Mg/Ca and $\delta^{18}Oc$ preclude salinity

reconstruction with a precision better than ±1.69 and hardly better than ±2.65, due to error propagation. Nevertheless, a direct linear fit to reconstruct salinity based on the same measured variables (Mg/Ca and $\delta^{18}Oc$) was established. This direct reconstruction of salinity lead to a much better estimation of salinity (±0.26) than the successive reconstructions.

I. INTRODUCTION

Since Emiliani's pioneering work (1954), oxygen isotope compositions recorded in fossil foraminiferal shells became a major tool to reconstruct past sea surface temperature. After Shackleton's seminal studies (1967, 1968 and 1974), it became clear that part of the signal reflected glacial-interglacial changes in continental ice volume and hence sea level variations. The oxygen isotope composition of foraminiferal calcite ($\delta_{18}O_c$) is thus controlled by the temperature of calcification (Urey, 1947; Epstein et al., 1953) but also by the oxygen isotope composition of seawater ($\delta_{18}O_w$)~~)~~. The relative contribution of these two factors cannot be deconvolved without an independent measure of the temperature at the time of calcification such as e.g. Mg/Ca (e.g. Nürnberg et al., 1996; Rosenthal et al., 1997; Rathburn and DeDeckker, 1997; Hastings et al., 1998; Lea et al., 1999; Lear et al., 2002; Toyofuku et al., 2000; Anand et al., 2003, al., Kisakurek et al., 2008; Duenas-Bohorquez et al., 2009, 2011; Honisch et al., 2013; Kontakiotis et al., 2016; Jentzen et al., 2018). The sea surface temperature (SST) reconstructed from Mg/Ca of foraminiferal calcite has, therefore, increasingly been used in combination with the $\delta_{18}O$ signal measured on the same material, to estimate $\delta_{18}Ow$, global ice volume and to infer past sea surface salinity (SSS) (e.g. Rohling 2000, Elderfield and Ganssen, 2000; Schmidt et al., 2004; Weldeab et al., 2005; 2007). These studies also showed that, because of error propagation, inaccuracies in the different proxies combined for the reconstruction of past sea water $\delta_{18}O$ and salinity obstruct meaningful interpretations. Hence, while there is an understandable desire to apply empirical proxy-relationships down-core, additional calibrations appear necessary to make reconstructions more robust. Calibrations using foraminifera sampled from surface seawater (0-10m deep), provide the best possibility to avoid most of the artefacts usually seen when using specimen from core tops or culture experiments for calibration purposes. Here, we report a calibration based on *Globigerinoides sacculifer*, which should now and will be referenced in this manuscript as *Trilobatus sacculifer* (Spezzaferri et al., 2015), from the Atlantic Ocean. Mg and Sr concentrations were measured on individual specimens with Laser Ablation-Inductively Coupled Plasma-Mass Spectrometry (LA-ICP-MS), while the oxygen isotope composition of the same tests as used for the elemental analyses was subsequently measured by Isotope ratio Mass Spectrometry (IRMS). Environmental parameters (temperature: T, salinity: S, dissolved inorganic carbon: DIC and alkalinity: ALK) but also the isotopic composition (O_{18w}) of the seawater the foraminifers were growing in, were measured. The primary objectives of this study are to test and improve the calibration of (1) both the Mg/Ca and oxygen isotope paleothermometer for *T. sacculifer*, a paleoceanographically relevant species; (2) evaluate the agreement between observed and predicted $\delta_{18}O_w$ and (3) test potential for SSS reconstructions of the Atlantic Ocean. Our results indicate that the best possible salinity reconstruction based on locally calibrated equations from the present study, only allowed reconstruction with an uncertainty of ±2.49. Such an uncertainty does not allow for viable (paleo)salinity data. This is subsequently confirmed by a Monte Carlo simulation, applied to test successive reconstructions in an 'ideal case', where explanatory variables are known. This simulation shows that from a pure statistical point of view, successive reconstructions involving Mg/Ca and $\delta_{18}Oc$ preclude salinity reconstruction with a precision better than ±1.69 and hardly better than ±2.65, due to error propagation. Nevertheless, a direct linear fit based on the same measured variables (Mg/Ca and $\delta^{18}Oc$), and leading to much better estimation of salinity (±0.26), could be established.

2. MATERIAL AND METHODS

2.1. Collection procedure

Foraminifera were collected between October and November 2005, on board of the research vessel Polarstern (ANT XXIII/1) during a meridional transect of the Atlantic Ocean (Bremerhaven/Germany - Cape Town/South of Africa; Fig. 1a). Foraminifera were continuously collected from a depth of ca. 10 m using the ship's membrane pump (3 m_3/h). The water flowed into a plankton net (125 µm) that was fixed in a 1000 L plastic tank with an overflow (Fig 1b). Every eight hours, the plankton accumulated in the net was collected. Temperature and salinity of surface seawater were continuously recorded by the ship's systems, and discrete water samples were collected for later analyses of total ALK, DIC and $\delta_{18}O_w$ (see Tab. 1). Plankton and water samples were poisoned with buffered formaldehyde solution (20%) and $HgCl_2$ (1.5 ml with $70 gL_{-1}$ $HgCl_2$ for 1 L samples), respectively. In total, more than seventy plankton samples were collected during the transect, covering a large range in both temperature and salinity. Specimens of *T. sacculifer* from thirteen ~~selected~~ stations, selected as to maximize temperature and salinity ranges, were picked and prepared for analyses.

Salinity, temperature, DIC, ALK and $\delta^{18}O_w$ data reported in this paper represent October/November values for the selected stations.

2.2. Description of species

Trilobatus sacculifer is a spinose species with endosymbiotic dinoflagellates inhabiting the shallow (0-80 m deep) tropical and subtropical regions of the world oceans. This species displays a large tolerance to temperature (14-32°C) and salinity (24-47) (Hemleben et al., 1989; Bijma et al., 1990). Based on differences in the shape of the last chamber of adult specimens, various morphotypes can be distinguished. Among others the last chamber can be smaller than the penultimate chamber, in which case it is called kummerform (kf). ~~This~~ species shows an ontogenetic depth migration ~~and~~ predominantly reproduces at depth around full moon (Bijma and Hemleben, 1993). Just prior to reproduction a secondary calcite layer, called gametogenic (GAM) calcite is added (Bé et al., 1982; Bijma and Hemleben, 1993; Bijma et al., 1994). Juveniles (<100µm) ascend in the water column and reach the surface after less than approximately 2 weeks. Pre-adult stages then slowly descend within 9-10 days to the reproductive depth. In our samples (collected between 0 and 10 m depth), *T. sacculifer* specimens have not yet added the Mg-enriched gametogenic calcite, which generally occurs deeper in the water column just prior to reproduction. Therefore, only the trilobus morphotype without GAM calcite is considered (230µm to 500µm) in this study, which limits the environmental, ontogenetic and physiological variability between samples and should be taken into account when compared to other calibrations based on core top and/or sediment trap collected specimens.

2.3. Seawater analysis

The DIC and ALK analyses of the sea water were carried out at the Leibniz Institute of Marine Sciences at the Christian-Albrechts University of Kiel~~,~~ (IFM-GEOMAR), Germany. Analyses were performed by extraction and subsequent coulometric titration of evolved CO_2 for DIC (*Johnson et al.*, 1993), and by open-cell potentiometric seawater titration for ALK (*Mintrop et al.*, 2000). Precision / accuracy of DIC and ALK measurements are 1 µmol kg^{-1} / 2 µmol kg^{-1} and 1.5 µmol kg^{-1} / 3 µmol kg^{-1}, respectively. Accuracy of both DIC and ALK was assured by the analyses of certified reference material (CRM) provided by Andrew Dickson from Scripps Institution of Oceanography, La Jolla, USA. Measurements of $\delta^{18}O_w$ were carried out at the Faculty of Geosciences, Utrecht University, Netherlands. Samples were measured using a GasBench II - Delta plus XP combination. Results were corrected for drift with an in-house standard (RMW) and are reported on V-SMOW scale, with a precision of 0.1‰ and accuracy verified against NBS 19 of 0.2‰ respectively. For reconstruction calculations $\delta^{18}O_w$ data were corrected to the PDB scale by subtracting 0.27‰ (*Hut*, 1987).

2.4. Carbonate analysis

2.4.1. Foraminiferal sample preparation

Under a binocular microscope, maximum test diameter of each specimen was measured and individual tests were weighed on a microbalance (METTLER TOLEDO, precision ±0.1µg). Since the foraminifera were never in contact with sediments, the rigorous cleaning procedure required for specimens collected from sediment cores, was not necessary. Prior to analysis the tests were cleaned following a simplified cleaning procedure: All specimens were soaked for 30 min in a 3-7% NaOCl solution (Gaffey and Brönniman, 1993). A stereomicroscope was used during cleaning and specimens were removed from the reagent directly after complete bleaching. The samples were immediately and thoroughly rinsed with deionised water to ensure complete removal of the reagent. After cleaning, specimens were inspected with scanning electron microscopy and showed no visible signs of dissolution. This cleaning procedure preserves original shell thickness and thus maximises data acquisition during laser ablation. Foraminifera were fixed on a double-sided adhesive tape and mounted on plastic stubs for LA-ICP-MS analyses.

2.4.2. Elemental composition analysis

For each station, 5–8 specimens were analysed. Their last chambers were ablated using an Excimer 193 nm deep ultraviolet laser (Lambda Physik) with GeoLas 200Q optics (Reichart et al, 2003) creating 80 µm diameter craters. Pulse repetition rate was set at 6 Hz, with an energy density at the sample surface of 1 J/cm^2. The ablated material was transported on a continuous helium flow into the argon plasma of a quadrupole ICP-MS instrument (Micromass Platform) and analysed with respect to time. Ablation of calcite requires ultraviolet wavelengths as an uncontrolled disruption would result from higher wavelengths. By using a collision and reaction cell spectral interferences on the minor isotopes of Ca (^{42}Ca, ^{43}Ca and ^{44}Ca) were reduced and interferences of clusters like $^{12}C^{16}O^{16}O$ were prevented. Analyses were calibrated against NIST (U.S. National Institute of Standards and Technology) 610 glass using the concentration data of Jochum et al. (2011) with Ca as internal standard. For Ca quantification, mass 44 was used while monitoring masses 42 and 43 as internal check. In the calcite, the Ca concentration was set at 40%, allowing direct comparison to trace metal/Ca from traditional wet-chemical studies.

Mg concentrations were calculated using masses 24 and 26; Sr concentrations were calculated with mass 88. One big advantage in using LA-ICP-MS measurements is that single laser pulses remove only a few nanometers of material, which allows high resolution trace elements profiles to be acquired (e.g. Reichart et al., 2003; Regenberg et al., 2006; Dueñas-Bohórquez et al., 2009, 2010, Hathorne et al., 2009; Munsel et al., 2010; Dissard et al., 2009; 2010a and b; Evans et al., 2013; 2015; Steinhardt 2014, 2015; Fehrenbacher et al., 2015; Langer et al., 2016; Koho et al., 2015; 2017; Fontanier et al., 2017; De Nooijer et al., 2007, 2014, 2017a and b; Jentzen et al., 2018, Schmitt et al., 2019; Levi et al., 2019). Element concentrations were calculated for the individual ablation profiles integrating the different isotopes (glitter software). Even though the use of a single or very few specimens, can be criticised when determining foraminifera Mg/Ca and δ_{18}O in order to perform paleoclimate reconstructions instead of more traditional measurements, Groeneveld et al., (2019) recently demonstrated that for both proxies, single specimen variability is dominated by seawater temperatures during calcification, even if the presence of an ecological effect leading to site-specific seasonal and depth habitat changes is also noticeable.

2.5. Stable isotope analysis

The specimens used for elemental composition analyses using LA-ICP-MS were subsequently carefully removed from the plastic stubs and rinsed with deionised water before measuring their stable isotope composition. Depending on shell weight, 2 to 3 foraminifera were necessary to obtain a minimum of 20µg of material, required for each analysis. Analyses were carried out in duplicate for each station. The results, compiled in table 2, represent average measurements. The analyses were carried out at the Department of Earth Sciences of Utrecht University (The Netherlands), using a Kiel-III -Finnigan MAT-253 mass spectrometer combination. The $\delta_{18}O_c$ results are reported in ‰ PDB. Calibration was made with NBS-19 (precision of 0.06-0.08 ‰ for sample size 20-100 µg, accuracy better than 0.2‰).

2.6. Statistical analysis

Within this manuscript, all statistical analyses with regards to elemental and isotopic data, were carried out using the program R with default values (R Development Core Team (2019).

3. RESULTS

3.1. Elemental composition

Overall values of the Mg/Ca and Sr/Ca ratios in the tests of ~~T.~~ *sacculifer* varied from 1.78 to 5.86 mmol/mol (Fig. 2a) and 1.41 to 1.52 mmol/mol (fig. 2b), respectively (Tab. 2). These Mg/Ca concentrations compare well with results found in literature for this species from either culture experiments, plankton tow, or surface sediment, growing at the same temperatures (e.g. Nürnberg et al., 1996; Anand et al. 2003, Regenberg et al., 2009, Fig. 3). Similarly, the overall variation in Sr/Ca-values reported in this study is comparable to that observed in core top and cultured *G. ruber* and *T. sacculifer* combined, for comparable salinity and temperature conditions, (varying between 1.27 to 1.51mmol/mol; e.g. Cleroux et al., 2008; Kisakürek et al., 2008; Dueñas-Bohórquez et al., 2009).

The relationship between measured temperatures and both Mg/Ca and Sr/Ca ratios were calculated using least square differences. Both show a good correlation with surface water temperature (Fig. 2, Tab. 3). The Mg/Ca ratio increases exponentially by 8.3%/°C (best fit) (Mg/Ca and Sr/Ca ratios given in mmol/mol):

$$\mathrm{Mg/Ca}=(0.42\pm0.13)\,\exp((0.083\pm0.001)*T[°\mathrm{C}]),\quad R^2=0.86 \quad \mathrm{pvalue}=2{,}9\mathrm{e}{-}06 \qquad \text{(equation 1)}$$

whereas Sr/Ca ratio increases linearly by 0.6%/°C (Fig. 2a and b), best fit:

$$\mathrm{Sr/Ca}=(0.009\pm0.002)*T+(1.24\pm0.05),\ R^2=0.67 \quad \mathrm{pvalue}=5.\mathrm{e}{-}04 \qquad \text{(equation 2)}$$

Combining Mg and Sr data for a non-linear multivariate regression allows improvement of the correlation with temperature, best fit:

$$T=-(27\pm15)+(8\pm1)*\ln(\mathrm{Mg/Ca})+(28\pm11)*\mathrm{Sr/Ca},\ \mathrm{pvalue\ Mg/Ca{:}}\ 2.10\text{^-}4 \qquad \text{(equation 3)}$$
$$R^2=0.92 \quad \mathrm{pvalue}=2.\mathrm{e}{-}04$$

Regression for the relationship between salinity and Mg/Ca ratios does not show any clear correlation (R_2=0.09, p-value=0.32). This is in good agreement with previous culture experiment~~s~~ studies which only report a minor sensitivity of Mg/Ca to salinity in planktonic foraminifera (e.g. Dueñas-Bohórquez et al., 2009; Hönisch et al., 2013; Kisakürek et al., 2008; Nürnberg et al., 1996). The correlation observed between Sr/Ca ratios and salinity (R_2=0.29, p-value=0.053) is better compared to that between Mg/Ca and salinity, but remains relatively weak. Nevertheless, recalculated regressions of Mg/Ca, incorporating salinity, show an improvement of the correlation with temperature, best fit:

$$\ln(\mathrm{Mg/Ca[mmol/mol]}) = (-5.02\pm2)+(0.09\pm0.009)*T+(0.11\pm0.05)*S,$$
$$R_2=0.91 \text{ pvalue} = 5e\text{-}06$$

This result is in good agreement with the recent study of Gray and Evans (2019), who reported the minor Mg/Ca sensitivity of *Trilobatus sacculifer* to salinity (3.6 ± 0.01% increase per salinity unit) and described, based on previously published culture experiments' data (Dueñas-Bohórquez et al., 2009; Hönisch et al., 2013; Kisakürek et al., 2008; Lea et al., 1999; Nürnberg et al., 1996), a similar fit allowing to assess the sensitivity of foraminiferal Mg/Ca of *T. sacculifer* to temperature and salinity combined.

$$\mathrm{Mg/Ca}= \exp(0.054(S-35) + 0.062T-0.24) \quad \text{RSE: } 0.51 \quad \text{Gray and Evans (2019)}$$

In order to compare both equations, Mg/Ca values from our study were used to reconstruct temperature and salinity using the fit established per Gray and Evans (2019), versus reconstructed temperature and salinity using our fit. The observed R_2 are then 0.99 and 0.48 for temperature and salinity, respectively. We can conclude, that if the equation of Evans and Gray is in perfect agreement with our equation with regards to the temperature parameter, this is not the case for salinity, which shows a strong difference between the two equations, most probably explained by the weak correlation of Mg/Ca to salinity.

3.2. Stable isotopes concentration

The $\delta_{18}O$ (PDB) values of the tests ($\delta_{18}Oc$) and of the seawater ($\delta_{18}Ow$) vary from -0.70 to -2.98‰ and from 0.74 to 1.25‰, respectively (Tab. 1 and 2). The relationship between temperature and the foraminiferal $\delta_{18}O$ (expressed as a difference to the $\delta_{18}Ow$ of the ambient seawater) was estimated with a linear least squares regression:

$$T = (11.82 \pm1.3) - (4.82 \pm0.45)*(\delta_{18}Oc - \delta_{18}Ow) [‰]; R^2=0.90 \qquad \text{(equation 4)}$$

The oxygen isotope fractionation ($\delta_{18}Oc - \delta_{18}Ow$) shows a strong correlation with *in situ* surface water temperature (linear increase of 0.17‰/°C).

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3.3. Comparison with previously established ~~*T.*~~ *sacculifer* temperature reconstruction equations

~~As mentioned above~~, average juvenile and pre-adult *T. sacculifer* specimen only spend between 9 to 10 days in surface waters. Therefore, measured *in situ* temperature is representative of the calcification temperatures. This is supported by the strong correlation between measured temperature and δ_{18}O analyses (R_2=0.90, equation 4), and measured temperature vs. Mg/Ca, (R_2=0.87, equation 1). Nevertheless, diurnal variations in temperatures cannot be discarded and may induce a slight offset between measured average temperature and mean calcification temperature.

For comparison, three Mg/Ca temperature calibrations for *T. sacculifer* were considered in this manuscript. The equation of Nürnberg et al. (1996) based on laboratory cultures, (2) the equation established by Anand et al. (2003) based on sediment trap samples and (3) the equation derived by Regenberg et al. (2009) based on surface sediment samples of the Tropical Atlantic Ocean. In each of these studies only *T. sacculifer* without SAC chamber were considered, (Tab. 3).

Similarly, in addition to equation 4 established in this study, three δ_{18}O based paleo-temperature equations for *T. sacculifer* were used for comparison with our data set: (1) Erez and Luz, (1983) and, (2) Spero et al. (2003), both based on cultured specimens, and (3) Mulitza et al. (2003) based on surface water samples (Fig. 4; Tab. 3).

3.4. Correlation between measured δ_{18}O/Salinity

Salinity and the oxygen isotope composition of surface seawater were measured for 23 stations located between 33°N and 27°S of the Eastern Atlantic Ocean (Tab. 4), including the thirteen stations represented in figure 1, where foraminifera were sampled. The $\delta_{18}O_w$-salinity relationship (equation 5) is plotted in figure 5.

$$\delta_{18}\mathrm{Ow} = (0.194\pm0.04)*S - (5.8 \pm1.5),\ R^2=0.53 \qquad \text{(equation 5)}$$

For comparison, the δ_{18}Ow-salinity relationship for the tropical Atlantic Ocean calculated by Paul et al. (1999) (from 25°S to 25°N) based on GEOSECS data, and by Regenberg et al. (2009), based on data from Schmidt 1999 (30°N–30°S), are plotted in the same figure. Temporal, geographical and depth differences in sampling, as well as analytical noise, are most probably responsible for the observed variations.

4. DISCUSSION

4.1. Intra-test variability

The Mg/Ca and Sr/Ca composition of foraminiferal calcium carbonate was determined using laser ablation ICP-MS of the final (F) chamber of size-selected specimen. Eggins et al., (2003) report that the Mg/Ca composition of sequentially precipitated chambers of different species (including *T. sacculifer*) are consistent with temperature changes following habitat migration towards adult life-cycle stages. As described for *T. sacculifer* in the Red Sea (Bijma and Hemleben, 1994), juvenile specimens (<100µm) migrate to the surface, where they stay about 9-10 days, before descending to the reproductive depth (80m). The addition of GAM calcite proceeds immediately prior to gamete release (Hamilton et al., 2008). The specimens considered in this study were collected between 0 and 10 meters depth, and GAM calcite was not detected. This limits the impact of variability due to migration, reduces potential ontogenic vital effects responsible for inter-chamber elemental variations (Dueñas-Bohórquez, 2010) and, avoids variability due to variable amounts of GAM calcite precipitated (Nürnberg et al., 1996). This is confirmed by the strong correlation (R^2=0.87) observed between our Mg/Ca-reconstructed temperature vs. measured surface temperature. In agreement with measurements on specimens from culture experiments (Dueñas-Bohórquez, 2009), Mg-rich external surfaces (GAM calcite) were not observed in our samples.

Because the diameter of the laser beam used in this study was 80µm, it represents a reliable mean value of elemental concentration of the last chamber wall, for every analysis of a single shell a full ablation of the wall chamber was performed (until perforation was completed). For comparison, results from traditional ICP-OES Mg/Ca analyses (Regenberg et al., 2009), electron microprobe (Nurnberg et al., 1996) and laser ablation ICP-MS (this study) are plotted in figure 3a and suggest comparable foraminiferal Mg/Ca ratios for *T. sacculifer* at similar temperatures.

4.2. Incorporation of Sr into Mg/Ca-Temperature calibrations

Combining Mg and Sr data to compute temperature was first suggested by Reichart et al. (2003) for the aragonitic species *Hoeglundina elegans*. It has been demonstrated that variables other than temperature, such as salinity and carbonate chemistry (possibly via their impact on growth rate) are factors influencing Sr incorporation into calcite (e.g. Lea et al., 1999, Dueñas-Bohórquez et al., 2009; Dissard et al., 2010a; Dissard et al., 2010b). The good correlation of Sr/Ca with temperature in our results (R_2=0.67, p value= 5.e-04, Fig 2b), also suggests that temperature exerts a major control on the amount of Sr incorporated into *T. sacculifer'* tests. However, Sr/Ca concentration also shows a correlation with salinity (R_2=0.29, p-value=0.053), which is not observed for Mg (R_2=0.09, p-value=0.32). Therefore, the incorporation of Sr into the Mg-T reconstruction equation might improve temperature reconstruction by accounting for the impact of salinity. It has recently been suggested that the Sr incorporation in benthic foraminiferal tests is affected by their Mg contents (Mewes et al., 2015; Langer et al.; 2016). However, as pointed out in Mewes et al., (2015), calcite's Mg/Ca needs to be over 30-50mmol in order to noticeably affect Sr partitioning. There is no obvious reason to assume that planktonic foraminifera should have a different Mg/Ca threshold. Therefore, with a concentration between 2 to 6 mmol/mol (Sadekov et al., 2009), the observed variation in Sr concentration in *T. sacculifer*' tests can be safely considered to be independent of the Mg/Ca concentrations. Hence, other environmental parameters such as temperature, salinity and/or carbonate chemistry, potentially via an impact on calcification rates, must control Sr/Ca values.

The standard deviation of measured temperatures versus reconstructed temperature was calculated for each of the three Mg-temperature equations established in this study. For equation (1), based on Mg/Ca only, SD= 1.37, for equation (3), based on both Mg/Ca and Sr/Ca, SD=0.98, and for equation (4), based on Mg/Ca ratio and salinity, SD=1.03. Incorporation of Sr into the Mg-Temperature reconstruction equation resulted in the standard deviation the closest to 1 (SD=0.98), indicating that this statistically improved reconstructions possibly by attenuating the salinity effect as well as potentially other environmental parameters such as variations in carbonate chemistry or the effect of temperature itself. Therefore, the combination of Mg/Ca and Sr/Ca should be considered to improve temperature reconstructions (Tab. 3). For the remainder of this discussion, and in order to compare our data with previously established calibrations for *T. sacculifer*, the equation based on Mg/Ca alone (equation 1) will be considered.

4.3 Comparison with previous *T. sacculifer* Mg/Ca-Temperature calibrations.

Mg/Ca ratios measured on *T. sacculifer* from our study show a strong correlation with measured surface water temperature (R_2=0.86, p value=2.9e-06) (Fig. 2a), increasing exponentially by 8.3% per °C. The relation with temperature (equation 1) is comparable to the one published by Nürnberg et al., (1996) and within the standard error of the calibration (Fig. 3a). This implies that the temperature controlled-Mg incorporation into *T. sacculifer* tests is similar under culture conditions as it is in natural surface waters. The equation established by Duenas-Bohorquez et al., (2010) based on *T. sacculifer* specimen from culture experiments integrates ontogenetic (chamber stage) effects. Even though incorporating the ontogenetic impact may improve temperature reconstructions based on Mg/Ca ratios, this is not routinely done for paleo-temperature reconstruction using *T. sacculifer*. Therefore, the equation of Nürnberg et al., (1996) is used in our study for comparison of various reconstruction scenarios.

A comparable regression (similar slope) has been established for *T. sacculifer* from tropical Atlantic and Caribbean surface sediment samples by Regenberg et al. (2009) (Fig 3a). This regression predicts Mg concentrations that are about 0.15 mmol/mol higher compared to our study. Because the Mg-T calibration from Regenberg et al. (2009) is based on sediment-surface samples, Mg concentrations were correlated with reconstructed mean annual temperatures. This potentially leads to an over or under-estimation of temperatures depending on the seasonality of the growth period and might explain the observed difference between the two regressions. Due to sample limitation, we analysed foraminifera from a wider size fraction (230µm to 500µm), compared to Regenberg et al. (2009) (355-400µm), introducing an additional bias between the two datasets (Duenas-Bohorquez et al., 2010; Friedrich et al., 2012). Finally, Regenberg et al. (2009), compiled data of samples from the tropical Atlantic and Caribbean Ocean, while we collected samples from the Eastern tropical Atlantic. All of these potential biases can easily explain the small discrepancy observed between our regression and the one from Regenberg et al., (2009). Interestingly, Jentzen et al., (2018), were able to compare Mg/Ca ratios measured on *T. sacculifer* from both surface sediment samples of the Caribbean sea and specimen sampled with a plankton net nearby. They observed a similar systematic increased Mg/Ca ratio in fossils tests of *T. sacculifer* (+0.7 mmol/mol-1) compared to living specimens, arguing that different seasonal signals were responsible for the observed difference. However, it is interesting to note that the Mg/Ca differences observed between living *T. sacculifer* (e.g. this study and Jentzen et al., 2018) and fossils specimens (e.g. Regenberg et al., 2009 and Jentzen et al., 2018) could also be explained by the presence of GAM calcite on *T. sacculifer* from sediment samples, as GAM calcite is enriched with Mg compared to pre-gametogenetic calcite precipitated at the same temperature (Nurnberg et al., 1996). If Jentzen et al., (2018) and Regenberg et al. (2009) do not describe the presence or absence of GAM calcite on *T. sacculifer* specimens analysed in their studies, a study on the population dynamics of *T. sacculifer* from the central Red Sea Bijma and Hemleben (1990) concluded that the rate of gametogesis increased exponentially between 300 and 400µm to reach a maximum of more than 80% at 355µm (sieve size =500µm real test length). It can therefore safely be assumed that the Mg/Ca difference between living specimens from the plankton and empty shells from the sediment is due to GAM calcite.

The Mg-Temp data obtained by Jentzen et al., (2018) is however, in good agreement with the equation established by Regenberg et al., (2009), and will therefore not be considered separately in this study. The overall strong similarity observed between our regression and the one from Regenberg et al. (2009), indicates nevertheless that Mg-temp calibrations established on *T. sacculifer* specimen from plankton tow, can be applied to *T. sacculifer* (without Sac) from the surface-sediment, even if these applications have to be considered with care and only on sediment samples showing no sign of dissolution.

In contrast, the equation of Anand et al., (2003) based on sediment trap samples, is appreciably different (Fig. 3b). This may be due to: (1) difference in cleaning and analytical procedures, (2) uncertainty in estimated temperature (3) addition of GAM calcite at greater depth. Anand et al., (2003) fixed the intercept of the exponential regression for *T. sacculifer* to the value obtained for a multispecies regression and subsequently recalculated for each species the pre-exponential coefficients. Using this approach their new equation for *T. sacculifer* is: Mg/Ca= 0.35 exp (0.09*T), which is identical to Nürnberg et al., (1996) and equation 1 from our study. Still, this implicitly assumes a common temperature dependence exists for all species, which is not realistic. To avoid *a priori* assumptions only the primary equation of Anand et al., (2003) (see Tab. 3) is considered in this study.

4.4. Comparison with previous δ^{18}O-Temperature calibrations.

As for Mg/Ca, the oxygen isotope composition also shows a strong correlation with measured surface water temperature (R^2=0.90). The *T. sacculifer* δ^{18}O-temperature equation of Spero et al., (2003), based on a culture experiment, is very similar to equation 4 in our study. However, sensitivity (slope) differs within the uncertainties calculated for equation 4. As no uncertainties are given for the Spero et al., (2003) equation, it is difficult to determine whether these equations are statistically different or not. In contrast, the equation of Mulitza et al., (2003), has a similar slope (within uncertainties) but a higher intercept (Fig. 4a). The equation of Erez and Luz, (1983) differs considerably from equation 4, for both slope and intercept parameters. Bemis et al., (1998) suggested a bias in the calibration due to uncontrolled carbonate chemistry during the experiments of Erez and Luz (1983) (a decrease in pH, e.g. due to bacterial growth in the culture medium or to a higher CO_2 concentration in the lab (air conditioners, numerous people working in the same room etc), would quickly lead to an increase in δ^{18}O of culture-grown foraminifera). This could explain the observed effect between our study (equation 4) and the calibration from Erez and Luz (1983). Although the equation of Mulitza et al., (2003) is also based on *T. sacculifer* collected from surface waters, their equation is significantly different from equation (4). This deviation could possibly be due to a difference in size fractions considered in the two studies (230 to 500 µm, and 150 to 700 µm for this study and Mulitza et al., (2003), respectively). Berger et al. (1979), already reported that large *T. sacculifer* tests are enriched in δ_{18}O relative to smaller ones (variation of 0.5‰ between 177 and 590µm). Similarly, in culture experiments, larger shells of *Globigerina bulloides* are isotopically heavier relative to smaller specimens (variation of approximatively 0.3‰ between 300 to 415µm, *Bemis et al.*, 1998). Jentzen et al., (2018) reported that: 'Enrichment of the heavier ^{18}O isotope in living specimens below the mixed layer and in fossil tests is clearly related to lowered in situ temperatures and gametogenic calcification'. Gametogenic calcite has been shown to enrich δ_{18}O signatures by about 1.0-1.4‰ relative to pregametogenic *T. sacculifer* (Wyceh et al., 2018). Finally, variation in light intensity (e.g. due to different sampling period and/or sampling location), may have influenced the δ_{18}O composition via an impact on symbiont activity (Spero and DeNiro, 1987). Bemis et al. (1998) demonstrated that in seawater with ambient [CO_{32-}], *Orbulina universa* shells grown under high light level (> 380 µEinst m_{-2} s_{-1}) are depleted in O_{18} by on average 0.33‰ relative to specimens grown under low light levels (20-30 µEinst m_{-2} s_{-1}). The different correlation between δ_{18}O and temperature reported by Mulitza et al., (2003) may be caused by size fraction differences, different sampling time, light intensity, differences in calcification depth or hydrography, or a combination of factors. These are all potential biases that could explain the steeper intercept observed by Mulitza et al., (2003) relative to our study.

5. Reconstructions

A few scenarios are considered in the following section, in which one, two or three proxy equations are combined to solve for salinity.

Three Mg/Ca-paleo-temperature equations (Nürnberg et al., 1996; Regenberg et al., 2009; and Anand et al., 2003) were used to compare "reconstructed" temperatures to the known *in situ* surface water~~s~~ temperatures. The mean foraminiferal Mg/Ca ratio measured at each of our stations was inserted into each of the three equation and solved for temperature (Fig. 3b.). The linear regression of reconstructed temperatures based on Nürnberg et al. (1996) overlaps almost perfectly with the theoretical best fit. This confirms that calibrations based on culture experiments (the primary geochemical signal recorded in the tests) are very well-suited for reconstructing surface water temperature. The regression from Regenberg et al., (2009) reconstructed surface temperature that are too warm. This is in agreement with the fact that the Mg/Ca ratio from surface sediment foraminifera are slightly higher than for living specimen (Jentzen et al. 2018). The offset increases with decreasing temperature (0.5˚C and 1.5˚C respectively at 30˚C and 16˚C). Finally, the reconstructed temperature using the equation from Anand et al. (2003), shows a strong systematic offset. Because the equation of Nürnberg et al., (1996) matched our measured temperatures almost perfectly, their equation will be used to analyse further reconstruction. Still, we acknowledge that downcore reconstructions will inevitably also involve GAM calcite and hence other calibrations established using specimens collected deeper in the water column or in the sediment should be better suitable. Similarly, three δ_{18}O-paleo temperature equations (Erez and Luz, 1983; Mulitza et al., 2003; Spero et al., 2003) were tested to reconstruct δ_{18}Oc-δ_{18}Ow. The equation of Erez and Luz, (1983), shows a significant systematic overestimation of δ_{18}Oc- δ_{18}Ow, and will therefore not be considered any further. Measured surface water temperatures at our 13 stations were inserted into the equations of Mulitza et al., (2003) and Spero et al., (2003) to derive δ_{18}Oc-δ_{18}Ow (Fig. 4). The δ_{18}Oc-δ_{18}Ow reconstructions based on the equation of Mulitza et al. (2003) and Spero et al. (2003), are both slightly more positive, than the theoretical best fit. In order to test the robustness of δ_{18}Ow reconstructions from paleoceanographic literature (e.g. Nürnberg and Groeneveld, 2006; Bahr et al., 2011), we use the reconstructed temperatures based on the Mg/Ca-paleo-temperature equation from Nürnberg et al., (1996) to predict δ_{18}Ow using measured δ_{18}Oc and the equations from Mulitza et al., (2003) and Spero et al. (2003). The reconstructed δ_{18}Oc-δ_{18}Ow from inserting the Mg/Ca temperature into these equations is slightly overestimated (0.5‰), but the offsets remain small enough to consider these as reasonable reconstructions.

Nevertheless, when reconstructing δ_{18}Ow by inserting the Mg/Ca temperature and measured δ_{18}Oc in both equations, the correlation coefficients of the linear regressions are weak (R^2 = 0.19 and 0.13 for Spero et al., 2003 and Mulitza et al., 2003, respectively) demonstrating that the reconstructed δ_{18}Ow is not very reliable, therefore no reconstruction of salinity using these equations will be further tested in this manuscript.

Nevertheless, to test the robustness of theoretical and empirical salinity reconstructions, we have the perfect data set at hand, as every parameter is known from *in situ* measurement or sampling. We will use the equations 1, 4 and 5 established in this study and presented in table 3, for demonstration purposes.

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$$\mathrm{Mg/Ca} = ae^{bT} \qquad \textbf{Eq. 1}$$

with a=0.42(±0.13) and b= 0.083(±0.001)

$$T = c + d(\delta^{18}Oc - \delta^{18}Ow) \qquad \textbf{Eq. 4}$$

with c=12.08(±1.46) and d=-4.73(±0.51)

$$\delta^{18}Ow = eS + f \qquad \textbf{Eq. 5}$$

with e=0.171(±0.04) and f = -4.93(±1.66)

Classically, from those equations it is possible to extract variables estimated from the observation *Mg/Ca* and $\delta^{18}Oc$ through the equations:

$$\hat{T} = \frac{1}{b}(\log(\mathrm{Mg/Ca}) - \log(\mathrm{a})) \qquad \textbf{Eq.1'}$$

$$\widehat{\delta^{18}Ow} = \delta^{18}Oc - \frac{1}{d}\left(\hat{T} - c\right) \qquad \textbf{Eq. 4'}$$

$$\hat{S} = \frac{1}{e}\left(\widehat{\delta^{18}Ow} - f\right) \qquad \textbf{Eq. 5'}$$

Given that $\hat{T}$ is estimated from the fit from Eq. 1' (fig. 3a) and $\widehat{\delta^{18}Ow}$ is estimated from Eq. 4', $\hat{S}$ is finally calculated from Eq. 5' (figure 5). Hence, the error in $\hat{S}$ is an accumulation of errors from successive fits. In this study the standard deviation of the fit between $\hat{S}$ and the measured salinity for the 13 stations is ±2.49 and the R² is 0.33 (p-value 0.04) (Fig. 6a and b). In conclusion, even the best possible salinity reconstruction based on locally calibrated equations 1, 4 and 5 from the present study only allows salinity reconstructions with a precision of ±2.49. In the modern Atlantic Ocean, and based on recent sea surface salinity estimation (Vinogradova et al., 2019), such a variability would not allow to distinguish water masses between 60°N to 60°S. Similarly, on a temporal timescale, given the regional salinity variations expected in most of the ocean over glacial-interglacial cycles is less than ±1, 2σ (Gray and Evans, 2019), such an incertitude on salinity reconstruction would not even allow to distinguish modern *versus* last glacial maximum water masses.

In the following steps, we quantify the error propagation more precisely. In simple cases, error accumulation in an equation can be assessed by calculating the partial derivatives and by propagating the uncertainties of the equation with respect to the predictors (Clifford, 1973). However, for complex functions the calculation of partial derivatives can be tedious. Here, error propagation related to $\hat{S}$ was computed by a Monte Carlo simulation, which is simple to implement (Anderson, 1976). It is important to note that the propagated error with a reconstructed salinity is a combination of fitting errors and errors associated with measurement inaccuracies (Mg/Ca and δ^{18}Oc). First, we will only consider the error related to the fitting procedure, (Eq. 1',4' and 5', assuming that variables (i.e. the data) are perfectly known without uncertainties). For example, the fitting error related to Eq. 4' is computed by fitting δ^{18}Ow from measured δ^{18}Oc and measured Temperature, i.e. the data are known and not approximated. This is done by adding random Gaussian noise, with standard deviation corresponding to the RMSE (Root Mean Square error) of each fit (respectively 1.32°C for Eq.1', 0.15‰ for Eq. 4' and 0.55 for Eq. 5'). The resulting standard deviation error for the reconstructed Salinity based on 10000 fits following the Monte-Carlo approach amounted to ±1.69 (each fit using sampling from random distributions defined above). Hence, ±1.69 is the smallest possible error for salinity reconstructions, using the three steps above, only due to its mathematics. We can also estimate the error propagation at each step: $\hat{T}$±1.32°C (Eq.1'), $\widehat{\delta^{18}Ow}$±0.45‰ (Eq.4') and $\hat{S}$±1.69 (Eq.5'). Now we will include the uncertainties related to estimating the variables using proxy data. Hereto, some Gaussian noises simulating the uncertainties of measured variables (Mg/Ca and δ^{18}Oc) were introduced with standard deviations taken from Table 2. The resulting standard deviation error increased to ±2.65. Therefore, it can be concluded that statistically speaking, $\widehat{\delta^{18}Ow}$ cannot be reconstructed to a precision better than ±0.45‰, while salinity cannot be reconstructed to a precision better than ±1.69 (fitting errors only) and, in reality hardly better than ±2.65 (full to error propagation).

Finally, to complete this analysis, a direct linear fit to estimate salinity using exp $(-\delta^{18}Oc)$ and Mg/Ca was performed and led to an error of ±0.26 and a $R^2 = 0.82$ (p-value 2.10_{-4}):

$$\hat{S} = -0.16(\pm 0.02)\, e^{-\delta^{18}Oc} + 0.28(\pm 0.1)\frac{Mg}{Ca} + 35.80(\pm 0.33)$$ (R_2=0.81, p-value ≈ 2.10_{-4}) **Eq. 6**

This demonstrates that the direct reconstruction using the exact same variables as those initially measured (Mg/Ca and $\delta^{18}Oc$), led to a much better estimation of salinity that the successive reconstruction.

Finally, to complete this analysis, a direct linear fit to estimate salinity using exp $(-\delta^{18}Oc)$ and Mg/Ca was performed and led to an error of ±0.26 and a $R^2 = 0.82$ (p-value 2.10_{-4}):

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This demonstrates that the direct reconstruction using the exact same variables as those initially measured (Mg/Ca and $\delta^{18}Oc$), led to a much better estimation of salinity that the successive reconstruction.

6. Implications

We analyzed shell Mg/Ca and Sr/Ca ratios, and δ_{18}O in *T. sacculifer* collected from surface water along a North-South transect of the Eastern Tropical Atlantic Ocean. We find a strong correlation between Mg/Ca ratios and surface water temperature, confirming the robustness of surface water temperature reconstructions based on *T. sacculifer* Mg/Ca.

Insertion of the Sr/Ca ratio into the paleo-temperature equation improves the temperature reconstruction. We established a new calibration for a paleo-temperature equation based on Mg/Ca and Sr/Ca ratios for live *T. sacculifer* collected from surface water:

$$T=(-27\pm15)+(8\pm1)*\ln(Mg/Ca)+(28\pm11)*Sr/Ca$$

Scenarios were tested using previously published reconstructions. Results were compared to reconstructions performed using local calibrations established in this study and therefore supposed to represent the best possible calibration for this data set:

(1) Mg/Ca ratios measured in *T. sacculifer* specimens collected in surface water allow accurate reconstruction of surface water temperature.

(2) δ_{18}Ow can be reconstructed with an uncertainty of ±0.45‰. Such δ_{18}Ow reconstructions remain a helpful tool for paleo-reconstructions considering the global range of variation of surface δ_{18}Ow (from about -7 to 2‰, LeGrande and Schmidt 2006;).

(3) In contrast, the best possible salinity reconstruction based on locally calibrated equations 1, 4 and 5 from the present study, only allowed reconstruction with an uncertainty of ±2.49. Such an uncertainty renders these reconstructions meaningless and does not allow for viable (paleo)salinity data.

This is confirmed by a Monte Carlo simulation, applied to test successive reconstructions in an 'ideal case', where explanatory variables are known. This simulation shows that from a pure statistical point of view, successive reconstructions involving Mg/Ca and δ_{18}Oc preclude salinity reconstruction with a precision better than ±1.69 and hardly better than ±2.65, due to error propagation.

Nevertheless, a direct linear fit to reconstruct salinity based on the same measured variables (Mg/Ca and $\delta^{18}Oc$) was established (Eq. 6) and presented in table 3. This direct reconstruction of salinity should lead to a much better estimation of salinity (±0.26) than the successive reconstructions.

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Table 1. Measured temperature, salinity, DIC, ALK, and δ^{18}Ow of the stations selected for this study (October/November 2005). Mean annual temperature per station (World Ocean Atlas, 2005).

Stations	Latitude	Longitude	Measured T°C (±0.05) Oct/Nov.	Mean annual T°C	Salinity (±0.05)	DIC (µmol/kg) precision 1µm/Kg accuracy 2 µm/Kg	Alkalinity (µmol/kg) precision 1.5 µm/Kg accuracy 4 µm/Kg	δ^{18}Ow (PDB) precision 0.1 ‰ accuracy 0.2 ‰
25	22°38.640'N	20°23.578'W	24.91	21.8222	36.63	2069	2391	1.1
29	18°8.088'N	20°55.851'W	26.09	22.6964	36.24	2037	2369	0.9
31	14°32.128'N	20°57.251'W	28.24	25.0457	35.78	2009	2330	0.8
35	10°23.424'N	20°4.869'W	29.73	26.7731	35.63	1982	2304	1.2
38	7°2.114'N	17°27.818'W	29.43	27.764	34.67	1929	2257	0.7
40	4°22.323'N	15°16.911'W	28.47	27.7331	34.35	1915	2214	0.8
42	2°15.702'N	13°33.854'W	27.56	26.9215	35.72	2002	2332	1.1
46	1°35.741'S	10°33.846'W	25.91	25.6623	36.13	2053	2346	1.0
49	4°44.752'S	8°6.641'W	24.59	25.6229	36.07	2057	2369	0.9
52	8°6.086'S	5°29.077'W	23.80	24.864	35.99	2062	2360	0.7
56	11°51.783'S	2°30.743'W	22.18	23.6074	36.38	2071	2387	1.0
62	17°59.620'S	2°25.321'E	19.11	21.2856	35.99	2100	2369	1.1
66	22°26.998'S	6°6.922'E	18.71	20.1148	35.68	2070	2349	1.0

Table 2. Mean elemental (Mg/Ca and Sr/Ca) and isotopic (δ18Oc) composition per station, measured in foraminiferal calcite in mmol/mol and ‰ PDB, respectively. Elemental and isotopic compositions were determined on the same material (n varying from 5 to 9 specimens per station); isotopic analyses were done in duplicate for each station. Mean δ18Oc-δ18Ow measured per stations in ‰ PDB.

Stations	Measured Mg/Ca mmol/mol	Measured Sr/Ca mmol/mol	Measured δ18Oc ‰ (V-PDB) precision 0.08‰	Measured δ18Oc-δ18Ow ‰ (V-PDB)	Recons. δ18Ow (Mulitza) ‰ (V-PDB)	Recons. δ18Ow (Spero) ‰ (V-PDB)	Recons. δ18Ow (this study) ‰ (V-PDB)
25	3.22 ± 0.51	1.53 ± 0.08	-1.76	-2.82	0.38	0.40	0.88
29	4.01 ± 0.24	1.52 ± 0.06	-1.75	-2.63	1.00	0.87	1.44
31	4.78 ± 0.37	1.56 ± 0.18	-2.51	-3.33	0.73	0.49	1.11
35	5.46 ± 0.38	1.59 ± 0.08	-2.35	-3.59	1.27	0.94	1.62
38	4.31 ± 1.14	1.58 ± 0.14	-2.89	-3.59	0.07	-0.10	0.49
40	4.07 ± 0.64	1.57 ± 0.07	-2.98	-3.78	-0.18	-0.32	0.25
42	3.79 ± 0.49	1.53 ± 0.08	-2.38	-3.44	0.21	0.12	0.67
46	3.92 ± 1.24	1.47 ± 0.07	-1.67	-2.66	1.02	0.91	1.46
49	2.99 ± 0.39	1.55 ± 0.11	-1.83	-2.74	0.10	0.16	0.62
52	2.97 ± 0.30	1.50 ± 0.03	-1.34	-2.08	0.57	0.64	1.09
56	3.31 ± 0.53	1.50 ± 0.03	-1.06	-2.10	1.15	1.15	1.65
62	2.20 ± 0.24	1.47 ± 0.07	-0.70	-1.76	0.38	0.64	0.99
66	1.66 ± 0.17	1.48 ± 0.09	-0.74	-1.75	-0.46	-0.02	0.23

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Table 3. Calibration equations for *T. sacculifer*.

Source			R²	p-values
Mg/Ca Relationship with Temperature				
This study	**Mg/Ca=0.42(±0.13)e^(T*0.083(±0.001))**	**Eq. 1**	**0,86**	**2.9e-06**
Nürnberg et al., 1996	Mg/Ca=0.37(±0.065)e^(T*0.091(±0.007))		0,93	
Anand et al., 2003	Mg/Ca=1.06(±0.021)e^(T*0.048(±0.012))			
Regenberg et al., 2009	Mg/Ca=0.6(±0.16)e^(T*0.075(±0.006))			
Sr/Ca Relationship with Temperature				
This study	**Sr/Ca=(0.0094±0.002)*T+(1.29 ± 0.05)**	**Eq. 2**	**0,67**	**5.e-04**
Mg/Ca and Sr/Ca Relationship with Temperature				
This study	**T=(-27±15)+(8±1)*ln(Mg/Ca)+(28±11)*Sr/Ca**	**Eq. 3**	**0,93**	**2 e-04**
Me/Ca Relationship with Temperature and Salinity				
This study (Mg/Ca)	ln(Mg/Ca)=(-5.10±2)+(0.09±0.009)*T+(0.11±0.05)*S		0,91	5.e-06
This study (Sr/Ca)	Sr/Ca = (1.81±0.5) + (0.008±0.002) T - (0.01±0.01)*S		0,71	0.002
$\delta_{18}O$ Relationship with Temperature				
This study	**T= 12.08(±1.46)-4.73(±0.51)*($\delta_{18}O_c$ -$\delta_{18}O_w$)**	**Eq. 4**	**0,88**	**1,6 e-06**
Erez and Luz, (1983)	T= 16.06(±0.549)-5.08(±0.32)*(δ18Oc -δ18Ow)			
Mulitza et al., (2003)	T= 15.35(±0.71)-4.22(±0.25)*(δ18Oc -δ18Ow)			
Spero et al., (2003)	T= 12-5.67*(δ18Oc -δ18Ow)			
measured $\delta_{18}O$ vs. measured Salinity (this study)	**$\delta_{18}O_w$ = (0.171±0.04)*S – (4.93 ±1.66)**	**Eq. 5**	**0.38**	**1,2 e-03**
direct linear fit to reconstruct salinity based on measured variables (Mg/Ca and $\delta_{18}O_c$)	**S = -0.16 (±0.02) e ^(- δ^$_{18}O_c$)+ 0.28 (±0.1) Mg/Ca+35.80 (±0.33)**	**Eq. 6**	**0.82**	**< 2e-04**

Table 4. Temperature, salinity and $\delta_{18}O_w$ of the stations used to determine the salinity/ $\delta_{18}O_w$ relationship (equation 5)

Stations	Latitude	Longitude	T°C(±0.05)	Salinity(±0.05)	δ_{18}Ow (SMOW) precision 0.1% accuracy 0.2%
19	33°20.14'N	14°38.45'W	22,09	36,83	1,3
21	30°23.42'N	16°24.99'W	23,01	36,91	1,4
23	25°20.68'N	18°4.17'W	24,87	37,01	1,8
25	22°38.64'N	20°23.58'W	24,91	36,63	1,3
29	18°8.09'N	20°55.85'W	26,09	36,24	1,1
31	14°32.13'N	20°57.25'W	28,24	35,78	1,1
35	10°23.424'N	20°4.869'W	29.73	35.63	1,5
36	9°5.71'N	19°14.21'W	29,29	35,63	1,1
37	7°43.88'N	18°5.42'W	29,25	34,92	1,0
38	7°2.11'N	17°27.82'W	29,43	34,67	1,0
39	5°49.51'N	16°29.68'W	29,34	34,34	1,0
40	4°22.32'N	15°16.91'W	28,47	34,35	1,1
42	2°15.70'N	13°33.85'W	27,56	35,72	1,3
43	0°57.53'N	12°33.06'W	26,48	36,05	1,3
46	1°35.74'S	10°33.85'W	25,91	36,13	1,3
47	2°17.53'S	10°1.35'W	26,16	36,2	1,2
49	4°44.75'S	8°6.64'W	24,59	36,07	1,2
51	6°55.67'S	6°24.31'W	24,28	36,01	1,1
52	8°6.09'S	5°29.08'W	23,8	35,99	1,0
56	11°51.79'S	2°30.74'W	22,18	36,38	1,3
62	17°59.62'S	2°25.32'E	19,11	35,99	1,3
66	22°26.99'S	6°6.92'E	18,71	35,68	1,3
69	25°0.20'S	8°17.16'E	18,19	35,64	0,9
72	27°2.39'S	10°35.53'E	18,5	35,64	1,0

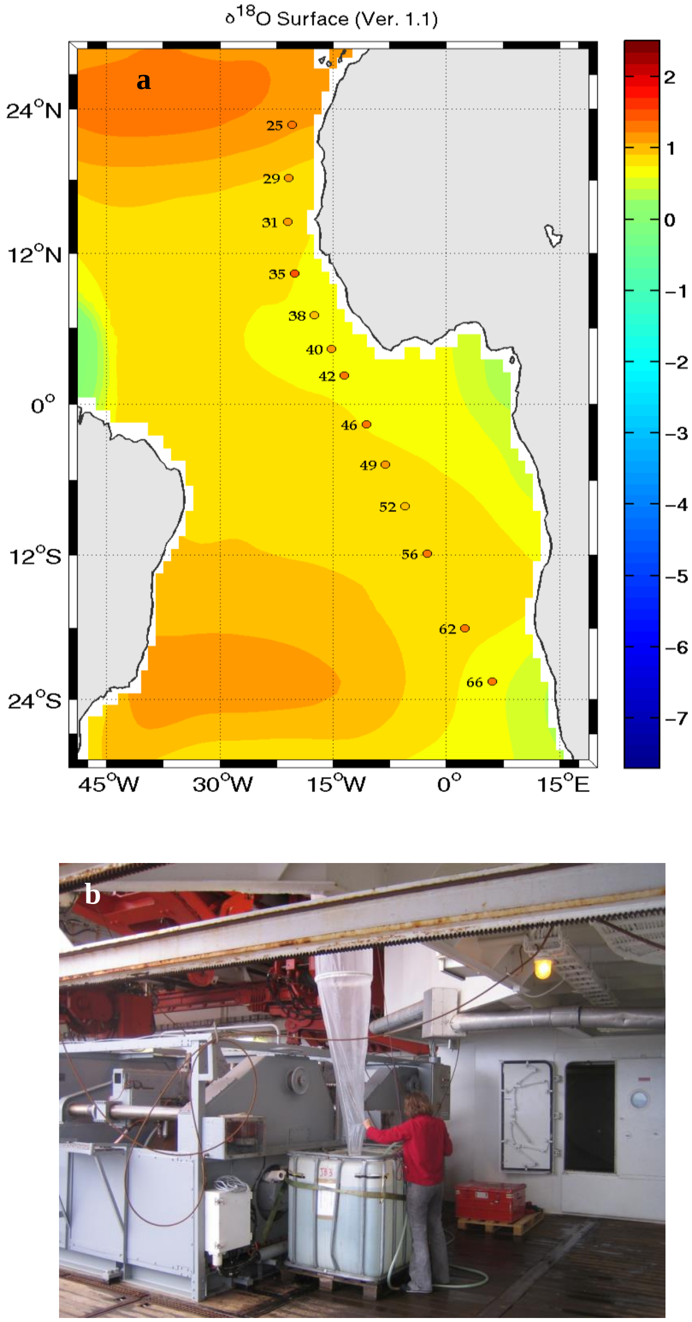
δ^{18}O Surface (Ver. 1.1)
a
24°N
12°N
0°
12°S
24°S
45°W
30°W
15°W
0°
15°E
25
29
31
35
38
40
42
46
49
52
56
62
66
2
1
0
−1
−2
−3
−4
−5
−6
−7
b

Figure 1

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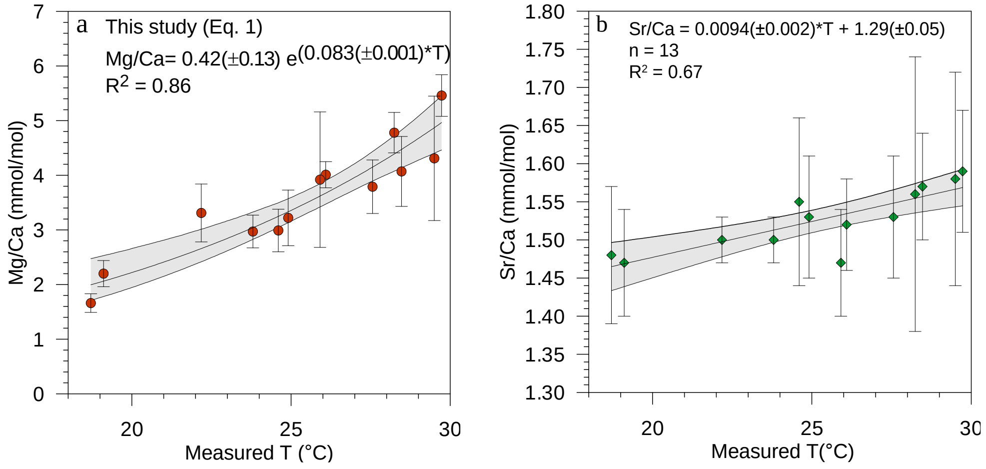

Figure 2

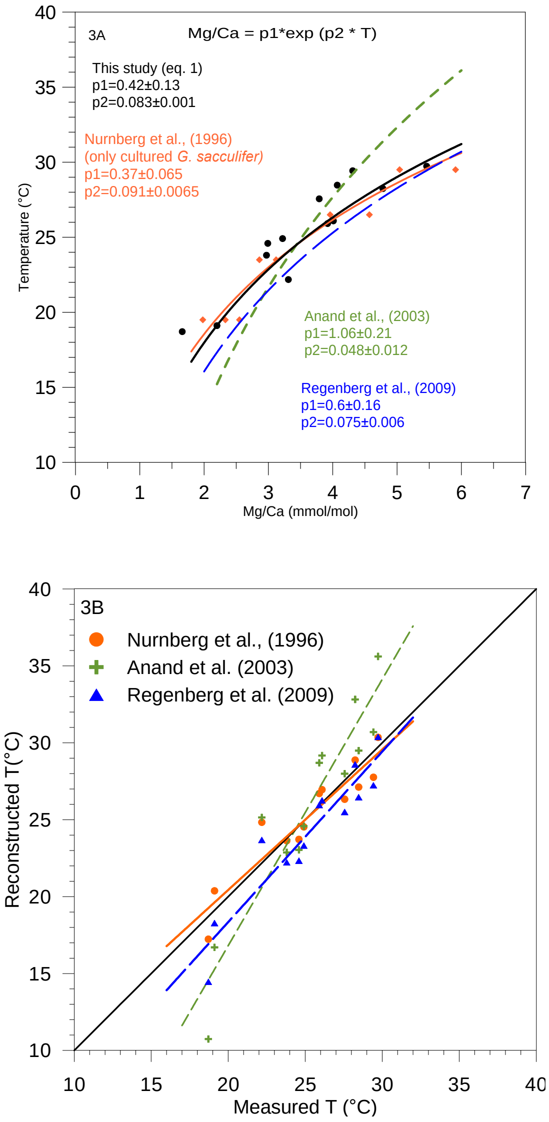
3A
Mg/Ca = p1*exp (p2 * T)
This study (eq. 1)
p1=0.42±0.13
p2=0.083±0.001
Nurnberg et al., (1996)
(only cultured *G. sacculifer*)
p1=0.37±0.065
p2=0.091±0.0065
Anand et al., (2003)
p1=1.06±0.21
p2=0.048±0.012
Regenberg et al., (2009)
p1=0.6±0.16
p2=0.075±0.006
Temperature (°C)
Mg/Ca (mmol/mol)
10
15
20
25
30
35
40
0
1
2
3
4
5
6
7
3B
Nurnberg et al., (1996)
Anand et al. (2003)
Regenberg et al. (2009)
Reconstructed T(°C)
Measured T (°C)
10
15
20
25
30
35
40

Figure 3

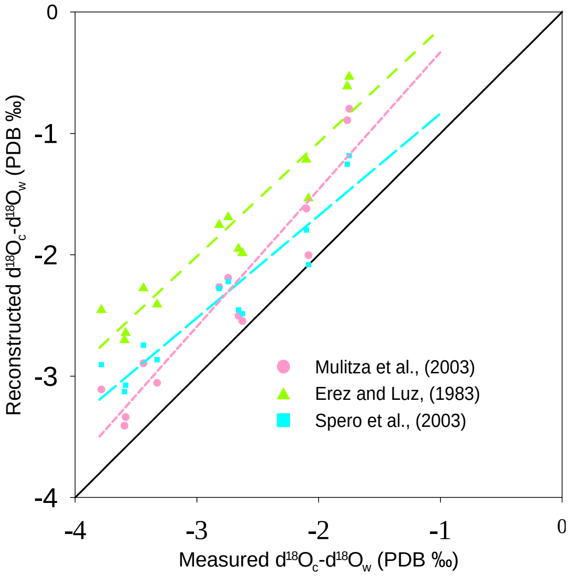
0
-1
-2
-3
-4
Reconstructed d18Oc-d18Ow (PDB ‰)
-4
-3
-2
-1
0
Measured d18Oc-d18Ow (PDB ‰)
Mulitza et al., (2003)
Erez and Luz, (1983)
Spero et al., (2003)

Figure 4

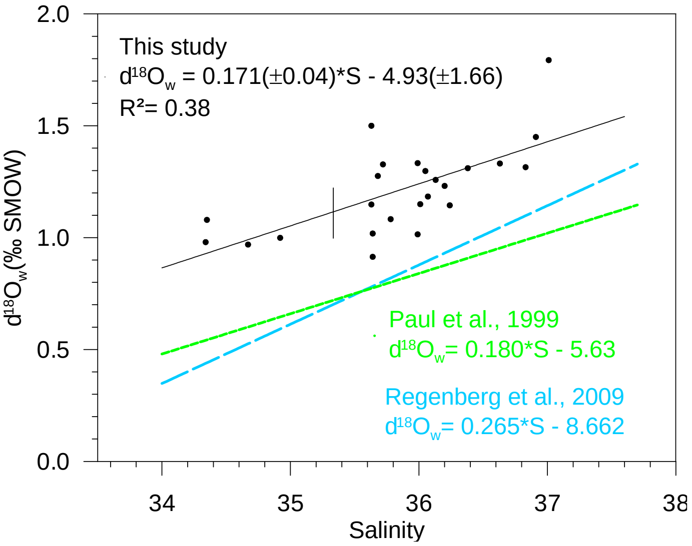
2.0
1.5
1.0
0.5
0.0
d18Ow(‰ SMOW)
This study
d18Ow = 0.171(±0.04)*S - 4.93(±1.66)
R²= 0.38
Paul et al., 1999
d18Ow= 0.180*S - 5.63
Regenberg et al., 2009
d18Ow= 0.265*S - 8.662
34
35
36
37
38
Salinity

Figure 5

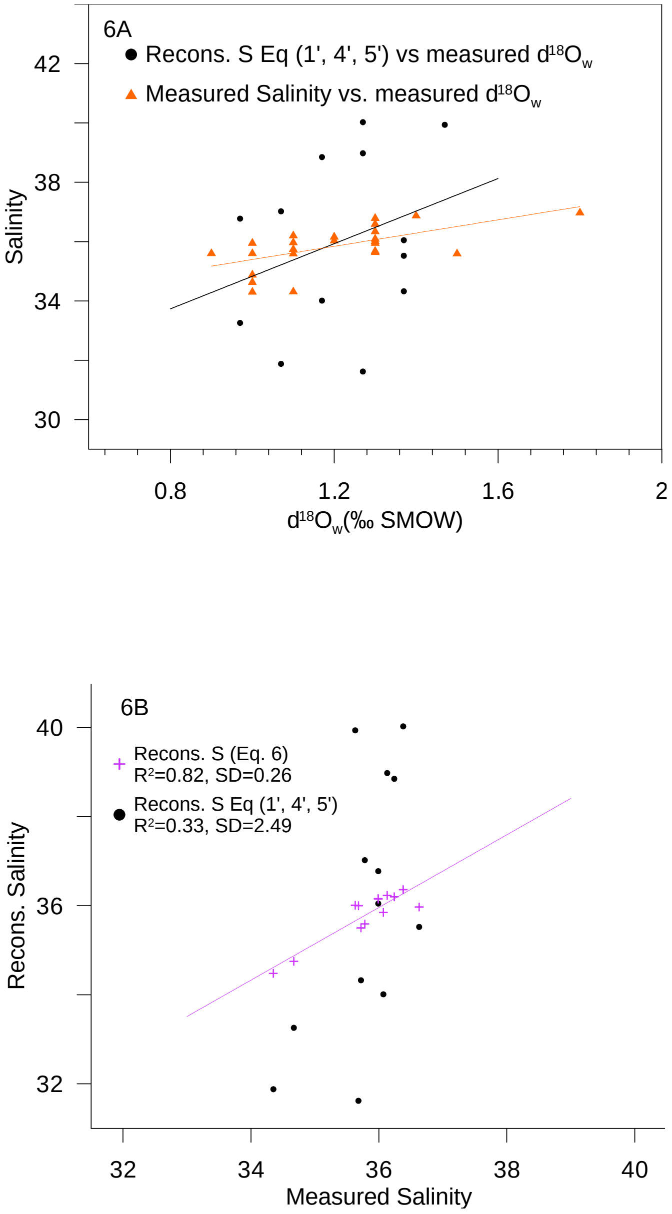
6A
Recons. S Eq (1', 4', 5') vs measured d18Ow
Measured Salinity vs. measured d18Ow
Salinity
42
38
34
30
0.8
1.2
1.6
2
d18Ow(‰ SMOW)
6B
Recons. S (Eq. 6)
R²=0.82, SD=0.26
Recons. S Eq (1', 4', 5')
R²=0.33, SD=2.49
Recons. Salinity
40
36
32
32
34
36
38
40
Measured Salinity

Figure 6

FIGURE LEGENDS

Fig. 1: Stations used in this study, plotted on gridded data set described in LeGrande and Schmidt (2006) (a). (http://data.giss.nasa.gov/o18data/grid.html). Set up for planktonic foraminifers collections (b).

Fig. 2: (a) Mg/Ca and (b) Sr/Ca (mmol/mol) and 95% confidence intervals plotted versus measured surface temperature (°C). Each point represents an average of the Mg/Ca and Sr/Ca per station.

Fig. 3 a) Mg/Paleo-temperature equations established in this study (equation 1) (black dots, and full lines), based on the data of Nürnberg et al., (1996) (Orange diamond and large full orange line); Anand et al., (2003) (small green dotted line) and Regenberg et al., (2009) (large blue dotted line) and **3b)** Reconstructed Mg-temperatures (Oct/Nov. 2005) plotted versus measured temperatures (°C) presented in Table 1. For each station mean measured Mg/Ca was inserted into the equation of Nürnberg et al., (1996) (only cultured specimens of *T. sacculifer*) (orange dots, full line), the equation of Anand et al., (2003) (green crosses, small dashed line), and the equation of Regenberg et al., (2009) (blue triangles, large dashed lines).

Fig. 4: Reconstruction of δ^{18}Oc-δ^{18}Ow by inserting the measured temperature into three δ^{18}O based paleo-T-equation: The equation of Spero et al., (2003) (light blue squares, large light blue dashed line), the equation of Mulitza et al., (2003) (pink dots, small pink dashed line), the equation sorted by Erez and Luz (1983) (green triangles, green dashed line) plotted versus measured δ^{18}Oc-δ^{18}Ow (‰ PDB). The diagonal line represents the 1:1 regression.

Fig. 5: Measured surface δ^{18}Ow (‰ SMOW) plotted versus measured surface salinity (stations listed in Tab. 4) (black dots and full line). Regression lines of the δ^{18}Ow-salinity relationship calculated by Paul et al., (1999) for the tropical Atlantic Ocean (from 25°S to 25°N) based on GEOSECS data (green line), and by Regenberg et al., (2009) (blue dashed line) based on Schmidt (1999) data for the Atlantic Ocean for the water depth interval of 0–100 m.

Fig. 6: a) Measured salinity (orange triangles) and reconstructed salinity based on equations 1, 4 and 5 from the present study (black dots), plotted versus measured δ^{18}Ow.

b) Reconstructed salinity based on 1) successive reconstructions using equations 1, 4 and 5 from the present study (black dots) and 2) direct linear fit (Eq. 6) based on the same measured variables (Mg/Ca and $\delta^{18}Oc$) (purple crosses), plotted versus measured salinity.