Herewith we submit a revised version of the manuscript entitled "Mg/Ca, Sr/Ca and stable isotope from planktonic foraminifera *T. sacculifer*: testing a multi-proxy approach for inferring paleo-temperature and paleo-salinity". We appreciate the effort the reviewers put into our manuscript, which greatly benefitted from their comments. Each of their comments is addressed separately below.

Answer to anonymous referee 1:

Comment 1: This text is of very high degree of interest for everyone who works on salinity reconstruction and understanding oxygen isotope/element ratio/salinity/temperature relation-ship. As said line 511, the authors "have the perfect data set at hand"!

One very important point is missing: the reader does not understand at which ontogenic stage foraminiferal specimen were chosen for Mg/Ca and δ 180 measurements. Are the studied specimen of *T. sacculifer* without SAC (in the paper called "kummer- form") considered as adults or pre-adults? so, do the author consider that *T. sacculifer* is adult when the SAC is built?

Answer:

Due to the very specific sampling strategy and as described from line 125 to 130: "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 in this study (230 μ m to 500 μ m), 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."

As described in this section none of the foraminifers considered in our study have GAM calcite nor a so called 'SAC-like chamber'.

Recently Poole and Wade (Journal of Systematic Palaeontology, 2019) published: "Many studies on extant forms group all morphospecies of the *T. sacculifer* plexus as *T. sacculifer*, or discern only between *T. sacculifer* 'with-sac' (i.e. *T. sacculifer* sensu stricto) and *T. sacculifer* 'without-sac' (i.e. *T. trilobus, T. immaturus* and *T. quadrilobatus*). In particular, palaeoceanographical studies utilizing *T. sacculifer* often avoid specimens possessing a sac-like final chamber as they may have different geochemical signatures or add variability (e.g. Spero & Lea 1993). **Equally,** *T. sacculifer* sensu stricto is often used to denote only *T. sacculifer* (i.e. only forms with a sac-like final chamber), whilst *T. sacculifer* sensu lato refers to all four morphospecies of the *T. sacculifer* plexus (regardless of whether a sac-like chamber is present or not)."

There is only one genotype of this species, now denoted *T. sacculifer*. The exact description of the different morphotypes (e.g. *sensu lato*) of *T. sacculifer*, is still a subject under discussion Therefore, we purposedly only described the sampling strategy and the samples that were analysed. It can be safely assumed that the analysed specimen are indeed pre-adult, without GAM calcite. As GAM calcite is produced **after** chamber formation has finished (including a final sac-like chamber or a

"kummerform" chamber) it can be inferred that we only analysed normal, (trilobus form) pre-gam specimens.

Same topic: the specimen size selected for measurement (cited line 316), is never explained - which test size the authors are talking about? The reader has to wait until line 393 to know this information. So, the description of the species and its ontogenic stages (chapter 2.2) should be a bit more precise.

Answer:

Selected test size fraction is described as early as line 128, but it is correct that the reason of the size selected for measurement is only explained line 316. To accommodate this comment, we have modified section 2.2 as follow:

Line 127-131...."Therefore, only the trilobus morphotype without GAM calcite is considered in this study, which limits the environmental, ontogenetic and physiological variability between samples even if a rather wide size fraction (230 to 500μ m) was selected due to sample size limitation. This should be taken into account when compared to other calibrations based on core top and/or sediment trap collected specimen."

The problem of the calcification depth of the last chamber of the selected individuals should also be addressed. In this paper, I feel like the authors follow an inverse reasoning (hypothetical causes form the basis of conclusions about reality). In Line 327-328, it is written: "This is confirmed by the strong correlation ($R^2=0.87$) observed between our Mg/Ca reconstructed temperature vs. measured surface temperature." I would write it (and think it) the other way around. The data set used for this paper is so nice, that the authors should start by the beginning = OK we don't know very well where the *T. Sacculifer* calcifies its test => first see how the correlation between "Mg/Ca reconstructed temperature" vs. "measured surface temperature" is. It is very strong. Conclusion =>

T. Sacculifer calcifies its last chamber at the sea surface (around 10m depth) !!!

Answer:

We understand the reviewer's comment and for clarity the statement line 323-334 was modified as follow:

"The specimens considered in this study were collected between 0 and 10 meters depth, and in agreement with measurements on specimens from culture experiments (Dueñas-Bohórquez, 2009), Mg-rich external surfaces (GAM calcite) were not observed in our samples. This indicates limited vertical migration (see section 2.2. for reproduction cycle), reducing therewith potential ontogenic vital effects responsible for inter-chamber elemental variations (Dueñas-Bohórquez, 2010) and, limited, if any, GAM calcite precipitation (Nürnberg et al., 1996). If the exact calcification depth of the last chambers of our *T. sacculifer* specimen can still be questioned, the lack of GAM-calcite, together with the strong correlation observed between measured surface temperature vs. Mg/Careconstructed temperature, support the idea that calcification of the last chamber of our specimen occurred around 10 meters depth. It should be noted that Lessa et al. (2020) recently confirmed that *T. sacculifer* calcifies in the upper 30 m."

The statement given line 448 and following (differences between Mulitza et al., (2003) equation and this study could possibly be due to a difference in studied size fractions) strengthens my

opinion that sizes and associated ontogenic stages are of primary importance in the conclusion of this study. It would have been best to normalize the element ratio and Oxygen isotope data with the corresponding individual test sizes.

Answer:

Our sampling strategy (underway pumping from ca. 10m depth), drastically reduced the 'possible' ontogenic stages at which our foraminifera were collected, which is confirmed by the complete absence of GAM calcite in our samples. This is, of course, not the case for studies based on foraminifera from surface-sediment, or sediment trap, where all ontogenic stages can be found, in abundance and therefore narrow size fraction can be considered.

However, the size fractions used by Mulitza et al. (2003) are even wider than ours. They state: ".... and includes measurements of various size fractions of foraminifera larger than 150 μ m." They further state: "Since our data agree with regression equations derived from culture experiments (Bemis et al., 1998; Spero et al., 2003), in which pH is controlled to be close to present-day surface waters, it is likely that the pH of calcification is the reason for the deviations."

The reviewer is right that normalizing the element ratio and oxygen isotope data to corresponding size fractions would have been preferable. Although not discussed in the current manuscript, this problem was considered during the elaboration of the paper, and Mg/Ca ratios determined on the last chamber of *T. sacculifer* tests, were reported against foraminifera test size, and are summarized in the table below. In this table, it appears that in our samples, varying size fractions do not have any clear impact on Mg/Ca ratios per station. Again, this is largely explained by our sampling strategy implying the collection of foraminifera that are seemingly all at the same "ontogenic" or "growth" phase, no matter what their variation in size might be (variation in size that can then be attributed to variation in temperature, light intensity and food availability). We are therefore confident that our results are not biaised by the sizes and associated ontogenic stages of the analyzed foraminifera. While answering this comment, we also corrected an error that occurred in line 165, as it is not 5-8 specimens that were analyzed per station, but a minimum of 5 to 8 specimen. The sentenced has now been corrected as follow: For each station 5-13 specimen were analysed.

For oxygen isotope data however, and because a minimum of 2 to 3 foraminifera were necessary to obtain enough material for analysis, it was impossible, due to limited sample size, to only measure foraminifera within a more restricted size fraction.

																										<u> </u>	
		Mg/Ca data measured per specimen per size fract											raction							-			-				
	Size fraction		25		29		31		35		38		40		42		46		49		52		56		62		66
																										1	
	< 212																					1	2,86				
	212-250	1	2,93					1	5,85	3	4,10	4	4,09													1	1,69
	250-300	3	3,11					3	5,38	5	4,36	4	4,05									2	3,03			5	1,65
	300-350	3	3,65	3	3,92	2		1	5,53					1	3,92							1	3,56	2	2,12	1	1,62
	350-425	2	3,38	2	3,84	3	5,04	1	5,26					6	3,68			3	2,93	2	2,69			3	2,25		
	425-500	2	3,22	1	3,62	1	4,55							2	4,05	3	3,94	2	3,07	2	3,20						
	> 500			7	4,28	4	4,70									4	4,36			2	3,04	1	4,05	1	2,18		
Total number of specimen analysed/st	ation	11		13		10		6		8		8		9		7		5		6		5		6		7	
Total Mean Mg/Ca per size fraction per	station		3,26		3,92		4,76		5,50		4,22		4,07		3,88		3,75		3,00		2,98		3,15		2,18		1,66
Total mean Mg/Ca per station			3,22		4,01		4,77		5,46		4,31		4,07		3,79		3,92		3,19		2,96		3,31		2,20		1,66

Mg/Ca ratios measured on the last chamber of T. sacculifer tests per station. In grey columns are reported the number of foraminifera analyzed per size fraction per station. In white columns are reported the mean measured Mg/Ca values per size fraction

per stations. In the bottom lines are summarized the mean Mg/Ca values per station as an average of size fraction mean values per stations. Below are reported mean Mg/Ca values per station.

In all calculations, I did not understand if the author have taken into consideration the precision error for in situ salinity measurements. Did the author estimate the quality of salinity data from the ship instrument (that effectively measures conductivity) by sampling sea waters for calibration purpose?

Answer:

As described line 103, temperature and salinity of surface seawaters were continuously recorded by the ship's systems, no extra samples were taken for calibration purpose, but yes the precision error for *in situ* salinity measurements (± 0.05) were taken into consideration.

See the attached pdf for details

Please also note the supplement to this comment: <u>https://www.biogeosciences-discuss.net/bg-2020-208/bg-2020-208-RC1- supplement.pdf</u>

All the extra comments listed within the manuscript have been incorporated in the final version.

Answer to the additional comments within the text:

-All exponents were properly written in the original manuscript, but when the article got transformed for the online version, exponents got changed. We'll pay attention to that before publication.

-The considered size fraction of our specimen is already given line 128.

- As suggested by the reviewer 'The last chamber' is now precised earlier in the manuscript: line74.

We thank reviewer 1 for this constructive review

Answer to anonymous referee 2:

Overall, I find this paper to be confusing, not overly novel, and missing key related studies: As the authors point out, their Mg/Ca-SST calibration results in a similar regression to studies published by Nurnberg et al. 1996.

Answer:

As pointed out in our manuscript line 401, our Mg/Ca-SST calibration results, are indeed, very similar to the regression by Nurnberg et al. (1996). However, we strongly disagree with the reviewer that our study is not overly novel, in the sense that the Mg/Ca-T°C calibration was previously published. On the contrary, being able to reproduce the same temperature-element regression based on foraminiferal geochemical signatures of very different samples: Regression based on experimentally cultured foraminifera maintained under laboratory conditions (Nurnberg et al., 1996) *versus* surface water foraminifera collected using underway pumping from ca. 10m depth (this study). As both studies use different analytical techniques (electron microprobe for

Nurnberg et al., 1996, *versus* LA-ICPMS for our study), we encourage and confirm the strong reliability of foraminifera Mg/Ca as a temperature proxy.

What makes this present study novel is their attempt to combine Mg/Ca and Sr/Ca measurements to further improve the SST calibration by accounting for the minor influence of salinity. However, it is not until section 4.2 that the basis for including Sr/Ca is explained. This should be put in the introduction of the paper, and more emphasis should be placed on this. Answer:

To accommodate this comment, the introduction from line 80 to 85 was modified as follow: "The primary objectives of this study are (1) to test and improve the calibration of both the Mg/Ca and oxygen isotope paleothermometer for the paleoceanographic relevant species *T. sacculifer;* (2) to test whether the incorporation of Sr into the Mg-T reconstruction equation improves temperature reconstruction by accounting for the impact of salinity; (3) to evaluate the agreement between observed and predicted $\delta^{18}O_w$ and (4) test potential for SSS reconstructions of the Atlantic Ocean."

I am concerned though because in lines 224-240, when Mg/Ca and Sr/Ca are combined, it is unclear how this is done. I do not understand how the combined regression was created, and how an R-squared of 0.92 is obtained.

Answer:

We understand the confusion, and even though our combined regression is correct, we modified the manuscript for better clarification as follows:

"The relationship between both Mg/Ca and Sr/Ca ratios and measured temperatures 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):

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

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

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

Concerning the temperature reconstruction, by inversing the approach, univariate regressions yields to:

 $T = (12.3 \pm 1.5) + ((10.5 \pm 1.2) * \log(Mg/Ca), R^2 = 0.86 \text{ pvalue} = 2,9e-06 \text{ (equation 1')}$ And

$$T = + (-84.1 \pm 22.9) + ((71.7 \pm 15)) * Sr/Ca, R^2 = 0.67$$
 pvalue=5e-04 (equation 2')

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

$$T=-(27\pm15)+(8\pm1)*\ln(Mg/Ca)+(28\pm11)*Sr/Ca, \text{ pvalue Mg/Ca: } 2.10^{-4}$$
 (equation 3)

 $R^2=0.92$ pvalue= 2.e-04

For comparison, with regression found in the literature, Mg/Ca is estimated below as a function of temperature and Sr/Ca.

$$Mg/Ca = \exp ((0.98 \pm 1.89) + (0.09 \pm 0.02)*T + (-1.43 \pm 1.45)* Sr/Ca)$$

R²=0.86 pvalue= 2.05e-05 (equation 3')"

The paper does not mention the Bayesian calibration for *T. sacculifer* from Tierney et al. (2019, Paleoceanography and Paleoclimatology). For completeness, I think an examination of this calibration should be included in the paper.

Also, the study of Gray and Evans 2019 is discussed on lines 260-266, but then not used in the comparisons later in the paper. Both of the calibrations for *T. sacculifer* from these two studies should be used later on in the paper when the different available calibrations are compared for "reconstructions".

Answer:

For completeness, both equation are now included and extensively discussed from line 263-286. Interestingly, both calibrations, when applied to our data, yield correlation coefficients of 0.9 for Gray and Evans (2019), and 0.82 for Tierney et al., (2019), only slightly below the correlation established in our study (R2 of 0.86, for T°-Mg/Ca only, 0.91 for T°C-Mg/Ca-S, and 0.93 for T°C-Mg/Ca-Sr/Ca). This is now described in line 283-285: "Here we can conclude, that despite the difference in sampling strategy and samples geographical distribution, our regression models are in line with the previous work of Gray and Evans (2019) and Tierney et al. (2019)."

There is no mention of the study by Thirumalai et al. 2016 (Paleoceanography and Paleoclimatology) that developed a program called PSUSolver that uses a similar Monte Carlo approach to propagate the error of Mg/Ca and δ 18Oc measurements for δ 18Osw convolution.

<u>Answer:</u> The similar technique (Monte Carlo approach) developed in the paper of Thirumalai et al. 2016 is now cited line 575 : "*Here, error propagation related to* \hat{S} *was computed by a Monte Carlo simulation, which is simple to implement (Anderson, 1976), and in line with the method applied by Thirumalai et al., (2019) on sediment samples. Ruber (W) specimen.*"

I find the section 5 on "reconstructions" to be confusing. The authors go through an exercise of trying to determine the best Mg/Ca calibration to use, and then use Nurnberg et al. for their "reconstruction". I do not understand why they do not use the Mg/Ca calibration they created in the current paper?

Answer:

The idea here is to test previously established calibrations, using our data, and compare the results with the measured environmental parameters (temperature) these fits reconstruct. Using our own calibration (established with our data), to test the fit to our data would be senseless.

I also find their use of "reconstruction" to be confusing. Paleoceanographers tend to use the term reconstruction for the creation of a long-term record. I think a term like "calibration testing" would make more sense for what the authors are trying to do.

The term "successive reconstructions" is also found throughout the paper, but I don't think this is the correct term.

Answer:

We disagree with the reviewer, in our study we use the same tools available to Paleoceanographers, to reconstruct the same environmental parameters. We therefore prefer to leave the terms originally chosen in the paper.

On lines 241 the authors discuss the relationship between Mg/Ca and Sr/Ca and salinity, but these relationships are not shown in any figures. I think these would be useful figures to include. Answer:

All the raw data are given in the table 1 and 2 of the manuscript, the correlation of Mg/Ca and temperature, and Sr/Ca and temperature, respectively are both shown on table 2, for conciseness no additional figure has been added to the manuscript.

The equation shown on line 250 should be solved for Mg/Ca and put into the same form as the equation on line 259 to enable comparison of the two equations.

Answer:

For completeness and to better enable comparison of equations, we now present both forms (equation 3 and 3') from line 243 to 249:

 $T=-(27\pm15)+(8\pm1)*\ln(Mg/Ca)+(28\pm11)*Sr/Ca, p value Mg/Ca: 2.10^{-4}$ (equation 3)

$$R^2=0.92$$
 pvalue= 2.e-04

For comparison, with regressions found in the literature, Mg/Ca is estimated below as a function

of temperature and Sr/Ca.

 $Mg/Ca = \exp ((0.98 \pm 1.89) + (0.09 \pm 0.02)*T + (-1.43 \pm 1.45)*Sr/Ca)$ R²=0.86 p value= 2.05e-05 (equation 3')

Lines 580-587 are a duplicated of lines 569-576.

<u>Answer:</u> We disagree with the reviewer, from line 569 to 576, we explain why we decide to use a Monte Carlo Simulation, and from line 580-587 we explain the two different applications of the simulation, first considering only the error associated with the successive fits (assuming that variables, i.e. the data, are perfectly known without any uncertainties), and then line 590 adding successively the uncertainties related to estimating the variables using proxy data.

Both these sections are necessary to understand how we proceed with the Monte Carlo simulation.

Table 2: it says 5 to 9 specimens per station but on line 165 it says 5 to 8 were used. Answer:

Both statements were corrected. 5-13 specimens were measured per sampling station (see answer to reviewer 1 where a table with Mg/Ca row data is given).

Throughout the whole paper, the 18 is δ 180 needs to be superscript.

Answer:

It was corrected in whole manuscript.

In table 1, it says World Ocean Atlas 2005 was used, but this is a quite old version of WOA. Answer:

The column showing annual surface temperature was removed from table 1, as it was of no use in this version of the manuscript.

In table 3 and 4, decimals should be used instead of commas.

Answer:

Commas were replaced by decimals within both tables 3 and 4.

Figure 1 – I think it would make more sense of a map of temperature was used rather than the gridded δ^{18} Osw product.

Answer:

The map was modified, and as suggested by the reviewer we changed the gridded δ^{18} Osw by surface temperature as a background to show the distribution of the sampling stations.

Also, the color bar needs to be labeled with units. I would also try to avoid using a "rainbow" colorbar.

<u>Answer:</u> The color bar is now labeled with units.

Figure 4 and 5: the d needs to be replaced with the delta symbol on the axis labels.

Answer:

The delta symbol is already present on the axis labels

The title of the paper does not seem to be grammatically correct. It needs the word "the" between "from" and "planktonic". I would also say δ^{18} O instead of "stable isotope" to make it more specific. <u>Answer:</u>

We agree with reviewer and have changed to "....THE PLANKTONIC FORAMINIFER...". However, we maintain "ISOTOPS" (now in plural) as Carbon isotopes were also measured, and will be made available in the raw data: "Mg/Ca, Sr/Ca AND STABLE ISOTOPES FROM THE PLANKTONIC FORAMINIFER *T. SACCULIFER*: TESTING A MULTI-PROXY APPROACH FOR INFERRING PALEO-TEMPERATURE AND PALEO-SALINITY"

list of all relevant changes made in the manuscript:

-We now explain in more details how Mg/Ca and Sr/Ca are combined and how an R-squared of 0.92 is obtained (line 224-249).

-Both the equation from Tierney et al. (2019, Paleoceanography and Paleoclimatology) and Gray and Evans (2019) are now applied to our data (line 263-286) which yielded to correlation coefficients of 0.9 for Gray and Evans (2019), and 0.82 for Tierney et al., (2019), only slightly below the correlation established in our study (R2 of 0.86, for T°-

Mg/Ca only, 0.91 for T°C-Mg/Ca-S, and 0.93 for T°C-Mg/Ca-Sr/Ca). This is now described in line 283-285.

-The study by Thirumalai et al. (2016) (Paleoceanography and Paleoclimatology) which uses a similar Monte Carlo approach to propagate the error of Mg/Ca and δ^{18} Oc measurements for δ^{18} Osw convolution, is now cited line 575.

- Regression combining Mg and Sr data to allow improvement of the correlation with temperature is now shown under both forms (equation 3 and 3') from line 243 to 249.

-The title was changed as follow: Mg/Ca, Sr/Ca AND STABLE ISOTOPES FROM THE PLANKTONIC FORAMINIFER *T. SACCULIFER*: TESTING A MULTI-PROXY APPROACH FOR INFERRING PALEO-TEMPERATURE AND PALEO-SALINITY.

Marked up manuscript version:

Mg/Ca, Sr/Ca AND STABLE <mark>ISOTOPES</mark> FROM <u>THE</u> PLANKTONIC FORAMINIFERA *T. SACCULIFER*: TESTING A MULTI-PROXY APPROACH FOR INFERRING PALEO-TEMPERATURE AND PALEO-SALINITY

Delphine Dissard (1, 2), Gert Jan Reichart (3, 4), Christophe Menkes (5), Morgan Mangeas (5), Stephan Frickenhaus (2) and Jelle Bijma (2)

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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 δ^{18} O signal from the same material, to provide estimates of δ^{18} O of the water (δ^{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, δ^{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 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. 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 δ^{18} O signal measured on the same material, to estimate δ^{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 δ^{18} O and salinity obstruct meaningful interpretations. Hence, while there is an understandable desire to apply empirical proxyrelationships 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 the last chamber of 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_w^{18}) of the seawater the foraminifera were growing in, were measured. The primary objectives of this study are (1) to test and improve the calibration of both the Mg/Ca and oxygen isotope paleothermometer for the paleoceanographic relevant species *T. sacculifer*; (2) to test whether the incorporation of Sr into the Mg-T reconstruction equation improves temperature reconstruction by accounting for the impact of salinity; (3) evaluate the agreement between observed and predicted $\delta^{18}O_w$ and (4) 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 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 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 m³/h). The water flowed into a plankton net (125 μ m) 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 seawaters 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 HgCl₂ (1.5 ml with 70gL⁻¹ HgCl₂ 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 $\delta^{18}Ow$ 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 in this study, which limits the environmental, ontogenetic and physiological variability between samples even if a rather wide size fraction (230 to 500µm) was selected due to sample size limitation. This should be taken into account when compared to other calibrations based on core top and/or sediment trap collected specimen

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 CO₂ 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 $\delta^{18}Ow$ 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, 5-13 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/cm². 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 (⁴²Ca, ⁴³Ca and ⁴⁴Ca) were reduced and interferences of clusters like ¹²C¹⁶O¹⁶O 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 for aminifera Mg/Ca and $\delta^{18}O$ 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 both Mg/Ca and Sr/Ca ratios and measured temperatures 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):

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

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

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

Concerning the temperature reconstruction, by inversing the approach, univariate regressions yields to:

 $T = (12.3 \pm 1.5) + ((10.5 \pm 1.2) \times \log(Mg/Ca), R^2 = 0.86 \text{ pvalue} = 2,9e-06 \text{ (equation 1')}$

And

 $T = + (-84.1 \pm 22.9) + ((71.7 \pm 15) * Sr/Ca, R^2 = 0.67 \text{ pvalue} = 5e-04 \text{ (equation 2')}$

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

$$T=-(27\pm15)+(8\pm1)*\ln(Mg/Ca)+(28\pm11)*Sr/Ca, pvalue Mg/Ca: 2.10^{-4}$$
(equation 3)
R²=0.92 pvalue= 2.e-04

For comparison, with regression found in the literature, Mg/Ca is estimated below as a function of temperature and Sr/Ca:

 $\frac{\text{Mg/Ca} = \exp ((0.98 \pm 1.89) + (0.09 \pm 0.02) * \text{T} + (-1.43 \pm 1.45) * \text{Sr/Ca})}{\text{R}^2 = 0.86 \text{ pvalue} = 2.05e \cdot 05 \text{ (equation 3')}}$

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 experiments 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:

Mg/Ca = exp ((-5.02 \pm 2)+(0.09 \pm 0.009)*T+(0.11 \pm 0.05)*S), R²=0.91 pvalue = 5e-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 ($3.6 \pm 0.01\%$ 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.

Mg/Ca= exp(0.054(S-35) + 0.062T-0.24) RSE: 0.51 Gray and Evans (2019)

Applying the equation of Gray and Evans (2019), to our data, leads to a correlation of 0.90, which is identical than our findings. In order to further 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 Gray and Evans (2019), 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<u>in our data</u>. Subsequently, the Bayesian model of Tierney et al. (2019) considering the group-specific core-top model for *T. sacculifer* was applied to our data. In that aim, Ω^{22} and pH, were calculated using Alk and DIC data presented in table 1. Because for aminifera in our studies were not submitted to cleaning protocol with a reductive step, the clean parameter was set to 0. It led to the following correlation:

$Mg/Ca = \exp(-11.66 + 0.06*T - 0.21 \Omega^{2} + 1.40 \text{pH}) \quad R^{2} = 0.82$

Here we can conclude, that despite the difference in sampling strategy and samples geographical distribution, our regression models are in line with the previous work of Gray and Evans (2019) and Tierney et al. (2019).

3.2. Stable isotopes concentration

The δ^{18} O (PDB) values of the tests (δ^{18} Oc) and of the seawater (δ^{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 δ^{18} O (expressed as a difference to the δ^{18} Ow of the ambient seawater) was estimated with a linear least squares regression:

$$T = (11.82 \pm 1.3) - (4.82 \pm 0.45)^* (\delta^{18} \text{Oc} - \delta^{18} \text{Ow}) \ [\%]; \ R^2 = 0.90 \qquad (\text{equation } 4)$$

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

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 (R²=0.90, equation 4), and measured temperature vs. Mg/Ca, (R²=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 for aminifera were sampled. The $\delta^{18}O_w$ -salinity relationship (equation 5) is plotted in figure 5.

$$\delta^{18}$$
Ow = (0.194±0.04)*S - (5.8±1.5), R²=0.53 (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 in agreement with measurements on specimens from culture experiments (Dueñas-Bohórquez, 2009), Mg-rich external surfaces (GAM calcite) were not observed in our samples. This indicates limited vertical migration (see section 2.2. for reproduction cycle), reducing therewith potential ontogenic vital effects responsible for inter-chamber elemental variations (Dueñas-Bohórquez, 2010) and, limited, if any, GAM calcite precipitation (Nürnberg et al., 1996). If the exact calcification depth of the last chambers of our T. sacculifer specimen can still be questioned, the lack of GAM-calcite, together with the strong correlation observed between measured surface temperature vs. Mg/Ca-reconstructed temperature, support the idea that calcification of the last chamber of our specimen occurred around 10 meters depth. It should be noted that Lessa et al. (2020) recently confirmed that T. sacculifer calcifies in the upper 30 m.

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 (R²=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 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 (230 μ m to 500 μ m), compared to Regenberg et al. (2009) (355-400 μ m), 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 $355 \mu m$ (sieve size =500 μm 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) addition of GAM calcite at greater depth and (3) uncertainty in estimated temperature, indeed, as mentioned in Gray et al., (2019): "Note the calibration line of Dekens et al. (2002) and Anand et al. (2003) does not fit the data of Anand et al. (2003) when climatological temperature, rather than

the $\delta^{18}O_{calcite} - \delta^{18}O_{water}$ temperature, is used. As shown by Gray et al., (2019), we show the calibrations of Anand et al (2003) are inaccurate due to seasonal changes in the $\delta^{18}O$ of sea water at that site.

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 preexponential 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 (R²=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 CO₂ 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 um 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 ¹⁸O 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 [CO₃²⁻], *Orbulina universa* shells grown under high light level (> 380 µEinst m⁻² s⁻¹) are depleted in ¹⁸O by on average 0.33‰ relative to specimens grown under low light levels (20-30 µEinst m⁻² s¹). 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 waters 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.

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 (R² = 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.

Mg/Ca =
$$ae^{bT}$$
 Eq. 1
with $a=0.42(\pm 0.13)$ and $b=0.083(\pm 0.001)$

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

with $c=12.08(\pm 1.46)$ and $d=-4.73(\pm 0.51)$

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

with $e=0.171(\pm 0.04)$ and $f=-4.93(\pm 1.66)$

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

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

$$\delta^{\widehat{18}Ow} = \delta^{18}Oc - \frac{1}{d}(\hat{T} - c) \qquad \text{Eq. 4}$$

$$\hat{S} = \frac{1}{e} \left(\delta^{\widehat{18}} O w - f \right)$$
 Eq. 5

Given that \hat{T} is estimated from the fit from Eq. 1' (fig. 3a) and $\delta^{\widehat{18}Ow}$ 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 $\pm 1, 2\sigma$ (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), and in line with the method applied by Thirumalai et al., (2019) on sediment samples G. Ruber (W) specimen. 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: $\hat{T}\pm 1.32^{\circ}$ C (Eq.1'), $\delta^{\widehat{18}}Ow\pm 0.45\%$ (Eq.4') and $\hat{S}\pm 1.69$ (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, $\delta^{\widehat{18}Ow}$ cannot be reconstructed to a precision better than $\pm 0.45\%$, 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 R² = 0.82 (p-value 2.10⁻⁴):

$$\hat{S} = -0.16(\pm 0.02) e^{-\delta^{18}Oc} + 0.28(\pm 0.1) \frac{Mg}{Ca} + 35.80(\pm 0.33) (R^2 = 0.81, \text{ p-value} \approx 2.10^{-4})$$
 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.

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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.

AKNOWLEDGEMENTS

We thank captain and crew of the Polarstern cruise ANT XXIII/1, (Bremerhaven-Cape Town) who have been of great support during this unforgettable experience. We are grateful to Susann Grobe of the Marine Biogeochemistry group of the IFM-GEOMAR (Germany) for measuring DIC and ALK of water samples. We thank Arnold Van Dijk of the Department of Earth Sciences-Geochemistry of the University of Utrecht (The Netherlands) for measuring oxygen isotope composition of water and foraminifera. We are thankful to Gijs Nobbe and Dr. Paul Mason for their support with LA-ICP-MS analyses. We would like to thank Beate Mueller (formaly Hollmann) for her technical support when handling foraminifera, and Dr. Gernot Nehrke, Dr. Stephan Mulitza, and Dr. Aurore Receveur for improving earlier versions of the manuscript. We thank Prof. Dieter Wolf Gladrow for his support during the initial draft of this manuscript. This work was supported by the German research foundation (DFG) under grant no. BI 432/4-2 ("PaleoSalt"), and by the European Science Foundation (ESF) under the EUROCORES

Programme EuroCLIMATE through contract No. ERAS-CT-2003-980409 of the European Commission, DG Research, FP6. Gert-Jan Reichart acknowledges funding from the program of the Netherlands Earth System Science Centre (NESSC), by the Ministry of Education, Culture and Science (OCW; Grant 024.002.001).

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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).

Suppri Ocean

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

Suppri

Table 2. Mean elemental (Mg/Ca and Sr/Ca) and isotopic (δ^{18} Oc) 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 13 specimens per station); isotopic analyses were done in duplicate for each station. Mean δ^{18} Oc- δ^{18} Ow measured per stations in ‰ PDB.

Stations	Measured	Measured	Measured	Measured	Recons.	Recons.	Recons.
	Mg/Ca	Sr/Ca	δ^{18} Oc ‰ (V-PDB)	δ^{18} Oc- δ^{18} Ow	δ18Ow (Mulitza)	δ18Ow (Spero)	δ18Ow (this study)
	mmol/mol	mmol/mol	precision 0.08‰	‰ (V-PDB)	‰ (V-PDB)	‰ (V-PDB)	‰ (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

Source		R ²	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	$Mg/Ca=0.6(\pm 0.16)e^{(T*0.075(\pm 0.006))}$		
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	$T=(-27\pm15)+(8\pm1)*\ln(Mg/Ca)+(28\pm11)*Sr/Ca$ Eq. 3	0.93	2 e-04
Me/Ca Relationship with Temperature and Salinity			
This study (Mg/Ca)	Mg/Ca=exp((-5.10±2)+(0.09±0.009)*T+(0.11±0.05)*S)	0.91	5.e-06
This study (Sr/Ca)	$Sr/Ca = (1.81\pm0.5) + (0.008\pm0.002) T - (0.01\pm0.01)*S$	0.71	0.002
δ ¹⁸ O Relationship with			
Temperature			
This study	$T = 12.08(\pm 1.46) - 4.73(\pm 0.51)^* (\delta^{18}O_c - \delta^{18}O_w) Eq. 4$	0.88	1.6 e-06
Erez and Luz, (1983)	$T = 16.06(\pm 0.549) - 5.08(\pm 0.32)^{*}(\delta 18\text{Oc} - \delta 18\text{Ow})$		
Mulitza et al., (2003)	$T = 15.35(\pm 0.71) - 4.22(\pm 0.25)^{*}(\delta 18Oc - \delta 18Ow)$		
Spero et al., (2003)	$T = 12-5.67*(\delta 18Oc - \delta 18Ow)$		
measured δ ¹⁸ O vs. measured Salinity (this study)	$\delta^{18}O_w = (0.171 \pm 0.04) * S - (4.93 \pm 1.66)$ Eq. 5	0.38	1.2 e-03
direct linear fit to reconstruct salinity based on measured variables (Mg/Ca and δ ¹⁸ O _c)	S = -0.16 (±0.02) e ^(- $\delta^{18}O_c$)+ 0.28 (±0.1) Mg/Ca+35.80 (±0.33) Eq. 6	0.82	< 2e-04

Table 3. Calibration equations for T. sacculifer.

Stations	Latitude	Longitude	T°C(±0.05)	Salinity(±0.05)	δ^{18} Ow (SMO) 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

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



Figure <u>1a</u>



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Figure 1b



Figure 2



Figure 3



Figure 4



Figure 5



FIGURE LEGENDS

Fig. 1: Stations used in this study, plotted on gridded data set <u>Reynolds et al., (2002)</u> (a). Set up	 Suppri
for planktonic foraminifera collections (b).	 Suppri
1 1	 Suppri

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.





a