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Development of coccolithophore-based transfer functions in the Western Mediterranean Sea: a sea surface salinity reconstruction for the last 15.5 kyr

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Abstract

A new dataset of 88 marine surface sediment samples and related oceanic environmental variables (temperature, salinity, chlorophyll *a*, oxygen, etc.) was studied to quantify the relationship between assemblages of coccolithophore species and modern en-

- vironmental conditions in the Western Mediterranean Sea and the Atlantic Ocean, west of the Strait of Gibraltar. Multivariate statistical analyses revealed that coccolithophore species were primarily related to the sea surface salinity (SSS) gradient, which explains an independent and significant proportion of variance in the coccolithophore data. A quantitative coccolithophore-based transfer function to estimate SSS was de-
- ¹⁰ veloped using the Modern Analog Technique (MAT) and weighted-averaging partialleast square regression (WA-PLS). The bootstrapped regression coefficient (R_{boot}^2) was 0.85_{MAT} and 0.80_{WA-PLS} , with root-mean square error of prediction (RMSEP) of 0.29_{MAT} and 0.30_{WA-PLS} (psu). The resulting transfer function was applied to fossil coccolithophore assemblages in the highly resolved (~ 65 yr) sediment core CEUTA10PC08
- ¹⁵ from the Alboran Sea (Western Mediterranean) in order to reconstruct SSS for the last 25 kyr. The reliability of the reconstruction was evaluated by assessing the degree of similarity between fossil and modern coccolithophore assemblage, and comparison of reconstruction with fossil ordination scores. Analogs were poor for the stadials associated with Heinrich Event 2 and 1 and part of the Last Glacial Maximum. Good analogs
- ²⁰ indicate more reliable reconstruction of the SSS for the last 15.5 kyr. During this period, several millennial and centennial SSS changes were observed and associated with variations in the Atlantic Water entering the Alboran Sea, sea-level oscillations, and arid or humid atmospheric conditions in the Western Mediterranean.

1 Introduction

²⁵ Coccolithophores are one of the major components of marine phytoplankton. They are sensitive to changes in many environmental variables, such as nutrients, temperature



and salinity and are widely used in qualitative paleoenvironmental studies (Baumann et al., 2005; Guerreiro et al., 2013, 2014). These studies provide general insight into the response of coccolithophores to environmental variables, but quantitative studies (e.g. transfer functions) allow assessing these relationships in a more rigorous and clear

- manner. Transfer functions are based on the calibration of the modern relationship between organisms and environmental conditions, and this information is in turn used to reconstruct past environmental variables. Different statistical approaches based on coccolithophores have been proposed in order to generate quantitative paleoreconstructions of different ecological variables. Giraudeau and Rogers (1994) used factor
- analyses and multiple regressions to estimate chlorophyll *a* from coccolithophore census counts in surface sediment samples in the Benguela upwelling area. Several authors (Beaufort et al., 2001, 1997; Incarbona et al., 2010) calibrated the relative abundance of the coccolithophore *Floriphaera profunda* in surface sediment samples with respect to primary productivity and reconstructed past variations of this parameter in
- the Indian and Pacific oceans and in the Central Mediterranean Sea. Saavedra-Pellitero et al. (2011, 2013) used linear regression methods to derive past SST estimates in the southeast Pacific Ocean from coccolithophore census counts and accumulation rates. Bollmann et al. (2009) and Bollmann and Herrle (2007) applied multiple linear regressions to morphometric measurements of the coccolithophore *Emiliania huxleyi* from such all balls distributed even and plendates exemples to actual allocations and accumulation and plendates.
- ²⁰ globally distributed core-top and plankton samples to obtain modern and past sea surface salinity (SSS) estimates.

To date, no coccolithophore-based transfer function has been applied in the Western Mediterranean Sea, a semi-enclosed basin situated at mid-latitudes (Fig. 1a). In this region evaporation exceeds precipitation plus runoff, such that water budgets tend to

²⁵ be balanced by the advection of relatively less saline Atlantic Water (AW) through the Strait of Gibraltar (Bèthoux, 1979). The AW flows eastward while mixing with Mediterranean water to form the Modified Atlantic Water (MAW) at the surface (100–200 m) (Millot, 1999). This distinctive feature affects the spatial distribution of some environmental parameters such as SST and SSS, leading to the development of well-defined



longitudinal gradients between the Atlantic Ocean and the Western Mediterranean in annual terms. In this confined basin, the estimation of changes in those environmental parameters is essential for determining Atlantic–Mediterranean water mass exchange through the Strait of Gibraltar in the past (Rohling and Bigg, 1998; Schmidt, 1998). This exchange depends on variations in the hydrological cycle, ice-volume effects, and Mediterranean circulation patterns, which have a thermohaline origin (MEDOCGROUP, 1970).

The aim of this study is to explore the potential of coccolithophores for the development of quantitative reconstructions in the Western Mediterranean Sea. We study the response of coccolithophore assemblages from surface sediment samples from

- the response of coccolithophore assemblages from surface sediment samples from Atlantic Ocean and Mediterranean Sea to environmental variables. The resulting calibration model (transfer function) for salinity was used to reconstruct SSS changes at high-resolution in the Alboran Sea (Fig. 1a) for the last 25 kyr. The reliability of the reconstruction was assessed by analysis of the similarity between fossil and modern coccolithophore assemblages, and fossil ordination scores. Finally, centennial and mil-
- lennial SSS changes are described and discussed, and compared to regional records of SST, organic matter preservation and continental aridity.

2 Materials and methods

2.1 Modern training set

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20 2.1.1 Surface sediment samples

Initially, 117 core tops located around a horizontal transect along the Western Mediterranean Sea and near the Gulf of Cadiz in the Atlantic Ocean were selected. They had been retrieved at varying water depths ranging from 70 to 2620 m during several oceanographic surveys and were stored at the University of Vigo and at the Core Repository of the Institute of Marine Sciences – CSIC in Barcelona. The first cm (or the



second, if the first was unavailable) of the 117 core tops was sampled, assuming that it essentially represents present-day conditions.

2.1.2 Environmental variables

Data on temperature (Locarnini et al., 2013), salinity (Zweng et al., 2013), chlorophyll *a* (Boyer et al., 2013), oxygen content and saturation (García et al., 2014a), nitrate, phosphate, and silicate (García et al., 2014b) were obtained from the 2013 World Ocean Atlas (WOA13), and mixed layer depth (Monterey and Levitus, 1997), total alkalinity (T_{ALK}) and total dissolved inorganic carbon (DIC) (Goyet et al., 2000) for the training set sites were taken 1° longitude by 1° latitude grid, using weighted averaged gridding by Ocean Data View (ODV) software (Schlitzer, 2014). Similarly, data on pH and carbonate (CO_3^{2-}) were calculated using the "derived variable" tool of ODV software. These data have been averaged annually and seasonally (for summer and winter) from 1955 to 2012 and were selected at 10, 20, 30, 50, 75, 100, 125, 150, 200 and 300 m water depth.

15 2.2 Fossil data set

The fossil coccolithophore data set used for the reconstruction comprises coccolithophore census counts from core CEUTA10PC08 (36°1′22″ N, 4°52′3″ W; 914 m b.s.l.) located in the Alboran Sea, previously published by Ausín et al. (2015). Fossil assemblages show good-to-moderate degree of preservation. Location of this ²⁰ core lies under the modern path of the AW at the surface, near the Strait of Gibraltar (Fig. 1a). Sediment core chronostratigraphy was based on 15 radiocarbon ages and covered the time span from 25 to 4.5 ka calibrated BP at a ~ 65 yr temporal resolution (Ausín et al., 2015). All dates reported in this study are given in calibrated ages BP.



2.3 Micropaleontological analyses

Both modern (surface sediment) and fossil (downcore) samples were prepared for coccolithophore analyses according to the techniques proposed by Flores and Sierro (1997). A polarized-light microscope at 1000× magnification was employed to iden-

- tify and count at least 500 coccoliths in each sample, belonging to 21 different taxa. Species whose relative abundance was < 1 % in the first count were considered later in 20 visual fields in order to estimate their abundance accurately. The final relative abundance of each species in each sample was then recalculated. *Gephyrocapsa* specimens smaller than 3 μm were lumped together and designated "small *Gephyrocapsa*"
- (Flores et al., 1997). The "medium *Gephyrocapsa*" group was made up of *Gephyrocapsa* whose size was between 3 and 5 μm. The following species were split according to the size criteria: *E. huxleyi* (< 4 and > 4 μm) and *Gephyrocapsa oceanica* (< 5 and > 5 μm). Other taxa identified in this study were *Calcidiscus leptoporus*, *F. profunda, Gephyrocapsa caribbeanica, Gephyrocapsa muellerae, Helicosphaera* spp., and *Syra-*
- cosphaera spp. (as dominant taxa). The rare taxa identified were Braarudosphaera bigelowii, Calciosolenia murrayi, Coccolithus pelagicus subsp. braarudii, Coccolithus pelagicus subsp. pelagicus, Oolithotus fragilis, Pontosphaera spp., Rhabdosphaera clavigera, Umbilicosphaera spp. and Umbellosphaera spp.

Twenty-nine samples were finally eliminated from the initial modern data set owing to their high content (> 10 %) in obviously reworked nannofossils. These taxa belong to older stratigraphic levels (consistently older than the Pliocene in this study), meaning that they were resuspended and transported from their original location to the sample site, and lack any relationship with modern environmental conditions. Therefore, the final training set (Supplement) comprised 88 surface samples (Fig. 1b): 78 from the

²⁵ Western Mediterranean (58 from the Balearic Sea and 20 from the Alboran Sea) and 10 from the Atlantic Ocean.



2.4 Statistical analyses

2.4.1 Relationship between coccolithophore assemblages and environmental variables

Prior to statistical analyses, environmental variables were checked for unimodal distribution. Only mixed layer depth, T_{ALK} and DIC were \log_{10} transformed, since transformation of other variables did not cause noticeable changes. Principal Component Analyses (PCA) was performed on this initial data set to assess the major environmental gradients and collinearity among the variables.

Coccolithophore relative abundances were square-root transformed to stabilize their variances. The species *Braarudosphaera* sp., *Calciosolenia* sp., *Coccolithus pelagicus* subsp. *braarudii, Coccolithus pelagicus* subsp. *pelagicus, and Pontosphaera* spp., were excluded from the modern (and consequently from the fossil) coccolithophore assemblages since their maximum relative abundance was not > 1 % in at least two samples. Detrended Correspondence Analysis (DCA) was then performed on the mod-

ern coccolithophore assemblage to estimate the length of the environmental gradient. A length of the first DCA axis > 2 Standard Deviation (SD) units indicates the unimodal responses of the organisms (Birks, 1995; ter Braak and Prentice, 1988), while shorter lengths indicate linear responses.

The Akaike's information criterion (AIC) was used in an ordination analysis to identify the minimum number of variables (subset) that, being statistically significant, explained the maximum variation in the modern coccolithophore assemblage. Canonical Correspondence Analysis (CCA) was used to evaluate the influence of this environmental subset to explain coccolithophore distribution in the modern training set.

The ratio between the first constrained axis and the first unconstrained axis (λ_1/λ_2) was used as diagnosis to test the strength of a single environmental variable when the effects of those remaining were excluded from the analyses (ter Braak and Juggins, 1993). If $\lambda_1/\lambda_2 \ge 1$, the variable under study is considered to be important one for explaining the distribution of the species. The proportion of the variance in the coc-



colithophore training set explained uniquely by each significant environmental variable was calculated using variance partitioning.

Ordination analyses and variance partitioning were performed using the "vegan" package v.2.3. (Oksanen et al., 2015) for R (R Development Core Team, 2015).

5 2.4.2 Transfer function

Calibration models were calculated for the variable of interest (and every variable by means of exploratory analysis) using the weighted-averaging-partial least squares (WA-PLS) (ter Braak and Juggins, 1993; ter Braak et al., 1993) and the Modern Analog Technique (MAT) (Prell, 1985), both implemented in C2 version 1.4.3 software (Juggins, 2007). All models were calculated for the cross-validation predictions by bootstrapping

- ¹⁰ 2007). All models were calculated for the cross-validation predictions by bootstrapping (999 permutation cycles) (Birks, 1995). In MAT, the number of analogs resulting in the maximum coefficient of determination (R_{boot}^2) between the observed and predicted values and the lowest root-mean square error of prediction (RMSEP) (Telford et al., 2004) was calculated using an optimization set together with the usual training and test sets
- ¹⁵ implemented in the "analoge" package for R (R Development Core Team, 2015). In WA-PLS, a decrease of 5 % or more in RMSEP was required to retain the next component (Birks, 1995; ter Braak et al., 1993).

Telford et al. (2013) reported that SST reconstructions based on planktonic foraminifera census counts calibrated at a fixed depth and for a particular season might

- ²⁰ be biased. The most suitable calibration should be based on the depth and season that most influenced the coccolithophore fossil assemblage from core CEUTA10PC08. These were determined by testing the statistical significance of the summer, winter, and annual reconstructions of the variable of interest at 10 different depths of the upper photic zone from 10 to 300 m, following the procedure described by Telford et al. (2013),
- using the "paleoSig" package v.1.1-1 (Telford, 2015) for R (R Development Core Team, 2015).

Outliers may reduce the power of prediction of the calibration model as well as introducing undesirable effects in model coefficients (Birks, 1995). Potential outliers were



determined as those whose absolute residual was higher than the mean SD of the observed values (Edwards et al., 2004).

A combination of the highest R_{boot}^2 and the lowest RMSEP was used as a criterion for the quality prediction of the model. The graphical representations of the observed values against the values predicted by the model and the residuals against the predicted values were used as a diagnosis of the model.

2.4.3 Derived reconstruction and evaluation

MAT and WA-PLS were applied to the fossil coccolithophore assemblages of core CEUTA10PC08, which were previously square-root transformed. In order to assess the quality of the modern analogs for the fossil (downcore) samples, the squared chord distance between each fossil sample and each sample in the modern training set (Overpeck et al., 1985) was calculated with MAT using C2 version 1.4.3 software (Juggins, 2007). A squared chord distance below the 10th percentile would be considered good, while values above this cutoff would represent assemblages with poor analogs (Simpson, 2007).

The first axis of the PCA analyses of the fossil dataset (PC1_{fossil}) shows the most important changes in the composition of the fossil coccolithophore assemblage. Comparison between PC1_{fossil} and the reconstructed variable of interest was used to assess whether the reconstruction could be considered representative of the major ecological changes of the fossil assemblage (Juggins, 2013).

3 Results

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3.1 Geographical distribution of coccolithophores

The geographical distribution of the main coccolithophore taxa is shown in Fig. 2. The relative abundance of *E. huxleyi* < $4 \mu m$ increases from the southern Spanish coast to the northern African coast, and high values are observed around the mouth of the Ebro



River Delta (Fig. 2a). By contrast, the small *Gephyrocapsa* group (Fig. 2b) shows the opposite distribution: a decreasing relative abundance from the Spanish to the African coast and low values near the Ebro River Delta. *E. huxleyi* < 4 µm and the small *Gephyrocapsa* group are small placoliths that on average constitute 83% of coccolithophore assemblages. *G. caribbeanica* and *F. profunda* (Fig. 2c and d) are more abundant in the Atlantic Ocean (up to 16 and 13%, respectively). *C. leptoporus* and *Helicosphaera* spp. (Fig. 2e and f) show patchy distributions and are more abundant (up to 7%) around the Catalan margin and the Balearic Islands. *G. muellerae* (Fig. 2g) is more abundant southeast of the Balearic Islands and shows a patch of 2% abundance in the northern part of the Alboran Sea. *G. oceanica* (< 5 µm) (Fig. 2b) is mostly distributed pear the

part of the Alboran Sea. *G. oceanica* (< 5 μm) (Fig. 2h) is mostly distributed near the Strait of Gibraltar, reaching up to 6% of relative abundance. It also shows a patch of 3% relative abundance around the Andarax River mouth (Figs. 1a and 2h).

3.2 Relationship between coccolithophores and environmental variables

The PC1 explains 56.1 % of the variance within the environmental data set (Fig. 3a) and is highly correlated to CO_3^{2-} , salinity, pH and T_{ALK} . PC2 explains 22.3 % of the total variance and summarizes primarily the information from temperature and phosphate.

The ordination based on the AIC determined that only salinity, nitrate, phosphate, silicate and oxygen are needed to explain the maximum variation in the modern coccolithophore assemblage and are significant at the 95 % level when added individually

- to the model via a forward selection procedure. The first axis of the DCA performed on the modern coccolithophore assemblage was 2.6 SD units. Accordingly, unimodal methods were followed. The CCA (Fig. 3b) reveals sites and species distribution along this environmetal subset. The others were also plotted as passive variables to avoid overfitting. Vectors reflect that salinity exhibits the longest gradient and is strongly cor-
- ²⁵ related with CCA1, indicating a strong relationship with coccolithophore distribution. Some sites from the Alboran and Balearic Sea and the taxa medium *Gephyrocapsa* and *E. huxleyi* (> 4 µm) are distributed along the CCA2. Individual CCAs (Table 1) to calculate λ_1/λ_2 show that salinity is the most important variable among those found



to be significant. Variance partitioning revealed that these significant variables account for 38.9% of the cumulative variance in the coccolithophore training set and salinity explains large proportion of this variance (15.5%).

3.3 Transfer functions

⁵ Salinity explained the largest amount of variation in the coccolithophore assemblages and consequently, was chosen to develop the coccolithophore-based transfer function. Additionally, comparison among the R_{boot}^2 from preliminary calibration models for each variable confirmed the best predictive power for salinity (Table 1).

Among the WA-PLS models for salinity, the two-component model (WA-PLS2) was chosen as the most suitable since it afforded a reduction of 6.4 % in the RMSEP. The ideal number of analogs for MAT was six.

The analyses of the amount of down-core variance explained by the summer, winter, and annual salinity reconstructions at 10 different depths and their statistical significance revealed that the mean-annual reconstruction at 10 m explained the highest variance. Hence, the reconstruction for core CEUTA10PC08 was based on the mean-annual salinity data at 10 m depth and referred to as SSS reconstruction.

Five samples showed higher residuals than the SD of salinity and were preliminary identified as potential outliers (Supplement). However, only one of these samples (CO-81-2/TK-2) was identified as outlier in both MAT and WA-PLS regression methods. This

²⁰ had a bright yellowish color under the microscope, likely due to the effect of diagenetic processes. In order to retain the maximum number of observations representing modern environmental conditions, only this sample was removed from subsequent model implementations, leading to an improvement of the MAT and WA-PLS2 R_{boot}^2 coefficient of 3.4 and 6.6 %, respectively, and reducing both Max_Bias_{boot} and RMSEP (Table 2).

Final MAT and WA-PLS2 models showed similar quality predictions (Table 2). The modern salinity gradient in the training set ranges from 36.2 to 38.2 psu. Intermediate values (37.1–37.6 psu) are less well represented by the observations (Fig. 4a). MATand WA-PLS2-predicted values are shown in Fig. 4b and c. The predicted vs. observed



values from both models approach the diagonal of slope one (that indicates perfect predictions) reasonably well (Fig. 4d and e). The residuals for MAT and WA-PLS2 models (Fig. 4f and g) are equally distributed around zero and show no apparent trends.

3.4 SSS reconstruction

⁵ The SSS reconstructions for core CEUTA10PC08 derived from both MAT and WA-PLS2 are very similar (Fig. 5a and b), with same range of SSS values. These only differ during the stadials associated with Heinrich Events 2 and 1 (H2 and H1), when the WA-PLS2-estimated SSS shows more pronounced salinity decreases.

The SSS reconstructions obtained from core CEUTA10PC08 (Fig. 5a) can be divided ¹⁰ into three intervals: (i) the period from 25.5 to 15.5 ka is characterized by higher values, ranging between 37.8 and 37 psu. Lower values are found from 20 to 18 ka followed by a drop of 0.8 psu at 17.3 ka, (ii) the period from 15.5 to 9 ka shows fast changes and large oscillations. An abrupt decrease from 37.9 to 36.9 psu is recognized at 15 ka, followed by large peaks of high values at 12.8, 11.1, and 10.2 ka; and (iii) the period from 9 to 4.5 ka records the lowest values, ranging between 37 and 36.5 psu and shows a general decreasing trend.

The errors associated with both SSS reconstruction are of a similar magnitude for the last 25 kyr (Fig. 5a). Squared chord distances between fossil and modern assemblages (Fig. 5b) revealed that many samples from 25.5 to 16 ka were above the 10th percentile. The comparison between $PC1_{fossil}$ and the SSS reconstruction is shown in Fig. 5c, showing general good agreement, especially for the last 16 kyr.

4 Discussion

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4.1 Geographic coccolithophore distribution and SSS

E. huxleyi (< 4 μ m) and *small Gephyrocapsa* (< 3 μ m) are very abundant (83% on ²⁵ average) and widespread in the Western Mediterranean (Fig. 2a and b) as previ-



ously reported for surface sediment samples in the Western Mediterranean by Álvarez et al. (2010). These taxa, especially *E. huxleyi* (< 4 μm), are cosmopolitan and tolerate wide ranges of temperature and salinity (Winter et al., 1994). The higher relative abundance of *G. caribbeanica, F. profunda* and *G. oceanica* in the Atlantic and the Mediterranean waters near the Strait of Gibraltar (Fig. 2c, d and h) suggests their preference for fresher waters. This notion is also indicated by the CCA (Fig. 3b), where these species are located on the right part of the salinity gradient. *C. leptoporus* (Fig. 2e) and *Helicosphaera* spp. (Fig. 2f) show higher abundances in the Balearic Sea and a similar spatial distribution. Nevertheless, the CCA (Fig. 3b) suggests that *Helicosphaera* spp.
have preference for more saline waters than *C. leptoporus*. This discrepancy might be related to the patchy spatial distribution of these species, possibly linked to the influence of common mesoscale structures in this area such as eddies or geostrophic fronts (Fig. 1a).

Salinity was highly correlated with CO₃²⁻ and pH (Fig. 3a and b). Carbonate chem-¹⁵ istry has already been found to be related to coccolith mass (Beaufort et al., 2011). Nevertheless, multivariate analyses revealed that salinity is significant and the most important variable of those studied in explaining coccolithophore data variance in this modern training set. Oviedo et al. (2015) have recently studied coccolithophore distribution from water column samples and in situ environmental measurement in the

- ²⁰ Mediterranean Sea. This study concluded that CO₃²⁻, pH and salinity are the most important factors in explaining coccolithophore data in the study area, which is in agreetment with our study. However, the individual importance and proportion of variance explained by each of these significant variables was not assessed in that study. Despite of this, the authors discarded salinity as a final explanatory variable arguing that
- *E. huxleyi* inhabits at a wide salinity range, suggesting a negligible ecological effect of salinity on coccolithophores. Contrary to this reasoning, the direct relationship between varying salinities and the morphology of *E. huxleyi*, the most abundant and ubiquitous extant coccolithophore (Cros and Fortuño, 2002), has been demonstrated by several authors (Bollmann and Herrle, 2007; Bollmann et al., 2009; Fielding et al., 2009; Green



et al., 1998; Paasche et al., 1996; Schouten et al., 2006), in both culture experiments and marine surface sediment samples. Nevertheless, findings by Oviedo et al. (2015) point toward the same direction of variability of coccolithophore assemblages in the Mediterranean Sea controlled by salinity and/or related variables. It is worth to mention that salinity influences solubility of CO₃²⁻ through several paths: the solubility of free carbon dioxide in water, the solubility product constants, the concentration of the ion hydrogen, and the quantity of calcium in the water (Trask, 1936). Based on this strong relationship, salinity could be influencing coccolithophore distribution through coccolith calcification processes. In contrast, Bollmann and Herrle (2009) have proposed an alternative hypothesis, suggesting that salinity influences coccolithophores through cell turgor regulation linked to osmotic processes.

Although there is no clear consensus about the mechanism through which salinity influence coccolithophore associations, many other studies point to a strong link between this variable and coccolithophore species. In the Japan Sea, salinity has been proposed

- to have an ecological or physiological influence on the production of alkenone and alkenoates, which are organic compounds mainly produced by *Emiliania* and *Gephyrocapsa* genus (Fujine et al., 2006). In the Baltic Sea, alkenone unsaturation ratios have been found to be significantly correlated with salinity (Blanz et al., 2005). In the Mediterranean Sea, Knappertsbusch (1993) studied the distribution of extant coccolithophore
- species in relation to in situ temperature and salinity data. A good correspondence was only found between coccolithophore species and the environmental parameters under study, indicating that *G. oceanica* was linearly correlated with salinity. Moreover, salinity has proven to be important to other marine unicellular planktonic groups such as diatoms (Fritz et al., 1991; Jiang et al., 2014; Li et al., 2012) and dinoflagellate cysts
- ²⁵ (Jansson et al., 2014, and references therein), reinforcing the hyposthesis of salinity as an important variable for planktonic communities in semi-enclosed basins.



4.2 Transfer function quality

A general good fit can be deduced for both models, although MAT was seen to perform slightly better from a higher R_{boot}^2 and a lower RMSEP (Table 2) and plotted predicted values compared with observed values (Fig. 4). The intermediate values of the salinity gradient are less well represented than the more extreme values (Fig. 4d and e). Unevenness can bias the RMSEP leading to overestimation of the predictive power of the model (Telford and Birks, 2011).While an even distribution would be always desirable, unevenness is a feature inherent to most training sets from oceanic environments. In this case, it is not severe and the observations, although unevenly distributed along the salinity gradient, do not leave gaps. The distribution of the residuals (Fig. 4f and g) indicates the adequacy of the model.

4.3 Downcore SSS reconstruction

The derived MAT and WA-PLS2 SSS reconstructions (Fig. 5a) are very similar. Nevertheless, WA-PLS2 shows more marked salinity decreases than MAT during the H2 (25.2–23.7 ka) and H1 (17.4–15.9 ka). Unlike WA-PLS, MAT does not consider the en-15 tire dataset when calculating the species optima, only the most taxonomically similar analogs, being more sensitive to local conditions (Telford and Birks, 2009). Fossil samples lack good analogs for the H2 and H1, coinciding with large peaks of E. huxleyi $(> 4 \mu m)$ (Fig. 5b). H2 and H1 have been linked to the entry of fresher water originating from the North Atlantic ice melting in the Western Mediterranean Sea (Cacho et al., 20 1999; Melki, 2011; Sierro et al., 2005), suggesting a link between the high abundances of *E. huxleyi* (> 4 μ m) and lower salinities in the past. By contrast, Bollmann and Herrle (2007) reported a significant current correlation between E. huxlevi (> 4 µm) and higher salinities from the study of globally distributed core-top samples. These authors used this relationship to estimate salinity values during the LGM. Interestingly, they 25 observed several overestimations with regard to other published values in samples characterized by high relative abundances of E. huxleyi (> 4 µm). These discrepancies



suggest that high percentages/presence of *E. huxleyi* (> 4 μ m) in the fossil record lacks modern analogs, as indicated by the high dissimilarity between fossil samples with high percentages of this species and modern samples (Fig. 5b).

Owing to MAT is strongly dependent upon on the analogs selected (Telford and Birks, 2009) and WA-PLS2 reconstruction for H2 and H1 is more coherent with a freshwater inflow scenario, it seems WA-PLS2 affords more reliable values than MAT. Consequently, WA-PLS2-estimated SSS is chosen for final interpretations.

Transfer functions assume that the ecological response of organisms to either the environmental variable of interest or to the linear combination of this important variable with others has not changed significantly over the time span represented by the fossil

- assemblage (Birks, 1995). The good agreement observed between PC1_{fossil} and reconstructed SSS patterns from 16 ka onwards (Fig. 5c) suggests that the SSS transfer function fulfills this assumption back to 16 ka. Larger differences are observed from 25 to 16 ka, possibly promoted by the situation of the absence of analogs during this
 period discussed above.
 - 4.4 SSS changes in the Alboran Sea over the last 15.5 kyr

The SSS reconstruction (Fig. 6a) might involve additional uncertainty during part of the LGM (from 25 to 18 ka), H2 and H1 derived from the lack of analogs. Consequently, the SSS reconstruction for that time span will not be discussed here.

20 4.4.1 Oldest Dryas

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An abrupt decrease in salinity of 0.8 psu occurred at 15.5 ka. This change is not supported by the findings of Fletcher and Sánchez Goñi (2008) or those of Combourieu Nebout et al. (2009) who, using pollen records from two sites in the Western Mediterranean, identified arid conditions in the southern Iberian Peninsula. The global sealevel rise of \sim 20 m during meltwater pulse 1A (mwp-1A) has been dated at 14.6 ka



(Bard et al., 1996; Weaver et al., 2003), simultaneous to the onset of the Bølling-

Allerød. Since this section covers 3000 yr with no control point (Fig. 6a), it could be an artifact of poorly constrained chronology for this time interval. Nevertheless, this seems unlikely since other authors (Duplessy et al., 1992; Emeis et al., 2000; Kallel et al., 1997) have reported similar abrupt SSS decreases in different regions of the Mediterranean Sea and the Atlantic Ocean at this time.

In particular, Duplessy et al. (1992) observed a SSS decrease of about 2.5 psu in the Atlantic Ocean west of the Strait of Gibraltar during the Oldest Dryas in northwestern Europe and related it to the meltwater release from the Barents and the Fennoscandinavian ice sheets. These authors also argued that such minor injections of freshwater would have been insufficient to trigger the observed drop in salinity, and proposed an additional feedback from changes in the hydrological cycle and water advection to promote changes in the thermohaline circulation and the observed changes in SSS.

4.4.2 Bølling-Allerød (B-A)

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The SSS values are generally low for the B–A, the Bølling being fresher than the ¹⁵ Allerød, both separated by the Older-Dryas (GI-1d) interval (Fig. 6a). Owing to the global sea-level rise during the B–A, and specifically during the mwp-1A between 13.5 and 14.1 ka, a greater volume of AW would have entered through the Strait, decreasing the average SSS. In addition, wetter conditions would have contributed to this freshening. Enhanced rainfall and increased river discharge have already been inferred from

- diatom assemblages, sediment grain-size, pollen records, elemental ratios and coccolithophore records in the Western Mediterranean during the B–A (Ausín et al., 2015; Bárcena et al., 2001; Combourieu Nebout et al., 2009; Frigola et al., 2008; Martínez-Ruiz et al., 2015; Rodrigo-Gámiz et al., 2011). This period of reduced salinity also coincides with the highest values of total concentration of C₃₇ alkenones, a proxy of or-
- ²⁵ ganic matter preservation (Cacho et al., 2002), from a nearby core located off the coast of Malaga (Ausín et al., 2015) (Fig. 6a and b), linked to the development of the Organic-Rich Layer (ORL-1) (Cacho et al., 2002). The ORL-1 appears in many sediment cores from the Alboran Sea as a consequence of the accumulation of high amounts of or-



ganic matter, although its origin is still under debate (Rogerson et al., 2008). Values below 37.25 psu match with an increasing trend in organic matter preservation. The joint effect of a salinity reduction of 0.8 psu and a temperature increase of $3^{\circ}C$ (Cacho et al., 2001) would have led to a significant reduction in sea surface density, possibly

- ⁵ prompting stagnation of the upper water column. Moreover, Ausín et al. (2015) observed a rise in primary productivity during this interval in the Alboran Sea from fossil coccolithophore assemblages. Frigola et al. (2008) and Martínez-Ruiz et al. (2015) identified a reduction in deep water formation in the Gulf of Lion using sediment-grain size analyses and elemental ratios, respectively. Increased organic matter export to
- the seabed, along with reduced deep-basin ventilation, would have hampered organic matter mineralization, reinforcing the formation of the ORL. Rogerson et al. (2008) have used model simulations to explore the mechanisms driving ORL formation. These authors concluded that a strong reduction in seawater density, which agrees with the decrease in reconstructed SSS from core CEUTA10PC08, in conjunction with a rise of
- the interface between deep and intermediate waters, would be the most likely explanation for the origin of the Alboran ORL.

The brief Intra-Alleröd Cold Period (IACP) (G1-1b) (Lehman and Keigmin, 1992) put an end to the low salinity values of the B–A. The SSS increasing trend is in agreement with the enhanced continental aridity reported for elemental ratios from a nearby core for this brief time span (Bodrigo-Gámiz et al. 2011)

²⁰ for this brief time span (Rodrigo-Gámiz et al., 2011).

4.4.3 Younger Dryas (YD) and the Holocene

The YD displays a shift from higher to lower SSS values, decreasing by 0.6 psu in total along its two phases (YDa and YDb). This is in keeping with a transition from arid to humid conditions observed in paleoclimate records from the Western and Central Mediter-

ranean Sea (Cacho et al., 2001; Combourieu Nebout et al., 2009; Rodrigo-Gámiz et al., 2011; Sbaffi et al., 2004). Several large short-term SSS fluctuations occurred as from the onset of the YD up to 8 ka (Fig. 6a). This time span coincides exactly with the highest summer insolation values of the last 25 kyr (threshold value above ~ 7 % of current



values), with a period of continuous SST increasing trend (Cacho et al., 2001) (Fig. 6c) and the rise in the post-glacial sea level (Fairbanks, 1989). However, fast SSS oscillations point to an intermittent influence of the forcing mechanisms. SSS changes in the Western Mediterranean can be driven by atmospheric and/or oceanic processes.

- ⁵ With regard to atmospheric conditions, pollen data from the Western Mediterranean (Combourieu Nebout et al., 2009; Dormoy et al., 2009; Fletcher et al., 2010) reveal the occurrence of periods of greater dryness, but they do not coincide exactly with SSS increases (Fig. 6a and d), as would be expected from reduced rainfall and decreased river discharge. Regarding oceanic processes, variations in the salinity and flux of the
- incoming AW are able to drive salinity changes in the study area (Bèthoux, 1979). Owing to its proximity to the Strait, core CEUTA10PC08 is expected to be a sensitive record to salinity changes in the past driven by AW influxes. Thus, periods of less saline AW influx should be recognizable in the SSS reconstruction. Six brief periods of a SSS decreasing trend were identified at 13.07–12.06, 11.95–11.71, 11.36–11.00, 10.09–9.83,
- 9.57–9.21, and 8.95–7.72 ka (Fig. 6a). Except for the period at 9.57–9.21 ka, all of them are accurately simultaneous to the brief Alboran cooling (AC) events (Table 3, Fig. 6c) that have been linked to North Atlantic influxes of cold atlantic waters in the Alboran Sea (Cacho et al., 2001). The synchronicity of the SST coolings and SSS freshenings suggests a common origin. AC events have been correlated with those of declining for-
- est (named APC) deduced from pollen analyses by Combourieu Nebout et al. (2009) (Table 3, Fig. 6a and d), suggesting increased aridity inland at times of freshwater advection events (FA; Table 3). The APC6 dry period from 9.6 to 8.9 ka does not match any AC event, but coincides with FA2 (Table 3), demonstrating the common nature of these short-term oscillations.
- ²⁵ The last freshening episode (FA1; 8.95–7.72 ka) includes the 8.2 ka event (Alley et al., 1997), which has been linked to a sub-thermocline freshening of 0.5 psu in the North Atlantic (Thornalley et al., 2009). However, no conspicuous changes are observed in reconstructed SSS at that precise time. Zanchetta et al. (2007) inferred episodes of increased rainfall from high-resolution oxygen isotopic records in a sta-



lagmite from the Corchia cave (central Italy). These authors found no evidence of the 8.2 ka event in relation to SSS. Similarly, we interpret that the 8.2 ka event would have had a negligible effect on surface salinity in the Alboran Sea. The aforementioned FA1 ends at 7.4 ka, when the lowest values SSS are recorded. At this time, the sea level in the Alboran Sea reached maximum high-stand conditions (Zazo et al., 2008). Moreover, the African Humid Period (AHP; 11–5.5 ka) affected the study area, especially up to 7.4 ka, when it started to decline (deMenocal et al., 2000; Renssen et al., 2003; Ritchie et al., 1985). The joint action of these processes certainly resulted in a decrease of SSS at 7.4 ka. From 7.4 to 4.5 ka, salinity values level off around 36.6 psu,

¹⁰ close to present SSS values in the Alboran Sea.

5 Conclusions

Multivariate statistical analyses show that coccolithophore distribution of modern coccolithophore assemblages in the Atlantic Ocean, west of the Strait of Gibraltar, and the Western Mediterranean was mainly influenced by annual mean salinity at 10 m ¹⁵ depth. MAT and WA-PLS2 calibration models show similar outcomes. These models were applied to coccolithophore assemblages from a fossil core to reconstruct SSS at high resolution for the last 25 kyr in the Alboran Sea. Statistical analyses reveal assemblages lacking good modern analogs in relation to the species *E. huxleyi* > 4 µm during H2 and H1 and part of the LGM, preventing further interpretations for these periods.

- A low SSS was found for the B–A, possibly due to the post-glacial sea-level rise and regionally wetter conditions in the adjacent continental areas. The consequent reduction in sea surface density is suggested to have triggered the formation of the ORL in the Alboran Sea. During the YD and Holocene, six brief, abrupt SSS decreases at 13.1–12.0, 11.9–11.7, 11.4–11.0, 10.1–9.8, 9.6–9.2, and 9.0–7.7 ka were linked to the
- advection of fresher and colder AW related to meltwater pulses in the North Atlantic and continental aridity. No evidence of the 8.2 ka event is found in the reconstructed SSS, which reached its lowest values at 7.4 ka, coinciding with high-stand conditions in the



Alboran Sea and the onset of the decline of the African Humid Period. SSS remained low from 7.4 to 4.5 ka, close to its present values.

A broader understanding of the ecological link between coccolithophore species and environmental parameters would be desirable in order to be able to place coccolithophore-based transfer functions within the ecological context in future works. Nevertheless, the diverse statistical tests performed in this study and the strong emphasis placed on assessing the validity and reliability of both the model and the reconstruction do reveal the potential of coccolithophores for developing transfer functions. The derived transfer function provides a potential independent proxy for quantitative reconstructions of SSS changes in other locations of the Western Mediterranean Sea over the last 15.5 kyr.

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Table 1. Multivariate analyses results. λ_1/λ_2 : individual CCA. Preliminar model coefficients from MAT and WA-PLS2. R_{boot}^2 : bootstrapped coefficient of determination between the observed and predicted values. RMSEP: root mean square error of prediction.

			MAT		WA-PLS	
Variable	λ_1/λ_2	% Explained	Boot_R ²	RMSEP	Boot_R ²	RMSEF
		variance				
Salinity*	1.38	15.47	0.83	0.30	0.75	0.33
Nitrate*	0.65	8.14	0.45	0.32	0.39	0.33
Phosphate*	0.25	4.89	0.36	0.02	0.19	0.02
Silicate*	0.22	8.93	0.56	0.24	0.40	0.26
Oxygen*	0.1	1.46	0.15	0.05	0.05	0.05
Chlorophyll a			0.61	0.05	0.58	0.05
Temperature			0.12	0.52	0.07	0.53
Oxygen Saturation			0.20	1.04	0.18	1.02
Mixed Layer Depth			0.31	0.19	0.25	0.19
CO_{3}^{2-}			0.74	0.02	0.70	0.02
рН [°]			0.70	0.02	0.67	0.02
TALK			0.70	0.00	0.67	0.004
DIC			0.51	13.31	0.48	13.16

* Variables determined by ordination based on AIC.

Table 2. Model coefficients from final MAT and WA-PLS2 cross-validated by boot-strapping
for SSS, after removal of one outlier. R_{hoot}^2 : bootstrapped coefficient of determination between
the observed and predicted values. Max_Bias _{boot} : bootstrapped maximum bias. RMSEP: root
mean square error of prediction (psu).

	MAT	WA-PLS2
R ² _{boot}	0.85	0.80
Max_Bias _{boot}	0.23	0.22
RMSEP	0.29	0.30



Table 3. Timing (given in ka cal. BP) of: freshwater advection events (FA) deduced from SSS decreases in core CEUTA10PC08 (this study); cooling events from core MD 95-2043 (ACYD-AC3, Cacho et al., 2001), and continental aridity periods from core ODP Site 976 (YD-APC5, Combourieu Nebout et al., 2009). All cores from the Alboran Sea.

SSS decreases	Cooling events	Continental aridity periods
FA6	ACYD	YD
13.07–12.06	13.1–12.0	12.8–11.75
FA5	AC6	APC9
11.95–11.71	11.9–11.65	11.75–11.4
FA4	AC5	APC8
11.36–11.00	11.21–10.95	11.0–10.8
FA3	AC4	APC7
10.09–9.83	10.34–9.95	10.5–9.8
FA2	-	APC6
9.57–9.21		9.6–8.9
FA1	AC3	APC5
8.95–7.72	9.08–7.56	8.5–7.9





Figure 1. Maps of the study area. **(a)** Location of core CEUTA10PC08 (red star). Black arrows trace general surface circulation. Legend: AW: Atlantic Water. MAW: Modified Atlantic Water. AC: Algerian Current. NC: Northern Current. **(b)** Location of the surface sediment samples in the study area. Maps generated with Ocean Data View software (Schlitzer, 2014).





Figure 2. Distribution of the main coccolithophore taxa considered in the training set studied according to their relative abundance (%) in the Western Mediterranean Sea and Atlantic Ocean: (a) *Emiliania huxleyi* (< 4 μ m). (b) small *Gephyrocapsa* (< 3 μ m) (c). *Gephyrocapsa caribbeanica*. (d) *Florisphaera profunda*. (e) *Calcidiscus leptoporus*. (f) *Helicosphaera* spp. (g) *Gephyrocapsa muellerae*. (h) *Gephyrocapsa oceanica* (< 5 μ m).





Figure 3. Multivariate analyses. **(a)** PCA based on the initial thirteen environmental variables. **(b)** CCA ordination plot with the site scores scaled by eigenvalues. The 88 sites are represented regarding their location in the Atlantic Ocean, Alboran Sea or Balearic Sea. Active and passive environmental vectors are represented by black and gray arrows, respectively. Scaling for the 16 taxa scores (open circles) is shown on the top left corner. mG: medium *Gephyrocapsa*; Eh (> 4): *Emiliania huxleyi* (> 4 µm); Eh: *Emiliania huxleyi*; sGg: small *Gephyrocapsa*; Gm: *Gephyrocapsa muellerae*; Go: *Gephyrocapsa oceanica*; sGo: small *Gephyrocapsa oceanica*; Rc: *Rhabdosphaera clavigera*; Sspp: *Syracosphaera* spp.; Of: *Oolithotus fraglis*; Gc: *Gephyrocapsa caribbeanica*; Hspp: *Helicosphaera* spp.; Cl: *Calcidiscus leptoporus*; Uspp: *Umbellosphaera* spp.; Ug: *Umbilicosphaera* spp.; Fp: *Florisphaera profunda*.





Figure 4. Diagnostic graphs of the models: (a) observed salinity values. (b) MAT-predicted salinity values. (c) WA-PLS2-predicted salinity values. (d) Observed *vs* MAT-predicted salinity values. (e) Observed *vs* WA-PLS2-predicted salinity values. (f) MAT-predicted salinity values *vs* residuals. (g) WA-PLS2-predicted salinity values *vs* residuals.





Figure 5. (a) SSS reconstructions for core CEUTA10PC08 derived from MAT (blue) and WA-PLS2 (green). The thin black lines represent the estimated values. The thick blue/green lines represent these original data fitted to a 3-point moving average smoothing spline. Pale blue/green shadows represent the error range, and dashed lines indicate current annual mean SSS in the Alboran Sea from the WOA13 (Zweng et al., 2013). (b) Dissimilarity between modern and fossil assemblages (black dots) measured by squared chord distance (left axis) plotted *vs* age. The red line indicates the 10th percentile. Relative abundance of the species *E. huxleyi* (> 4 μ m) (%; right axis). (c) Profiles comparing the PC1_{fossil} (black line) and WA-PLS2-estimated SSS (green line).





Figure 6. Paleoenvironmental records in the Alboran Sea: **(a)** WA-PLS2-SSS reconstruction (psu) for core CEUTA10PC08. Triangles stand for age control points. **(b)** C37 Alkenones (ngg⁻¹) from core HER-GC-T1 (Ausín et al., 2015). **(c)** SST (°C) from core MD95-2043 (Cacho et al., 2001). Red boxes represent the Alboran cooling events (AC). **(d)** Pollen record (%) from ODP Site 976 (Combourieu Nebout et al., 2009). Horizontal black lines cover the timing of periods of continental aridity (APC).

