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A nonlinear multi-proxy model based on manifold learning to reconstruct water temperature from high resolution trace element profiles in biogenic carbonates

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Abstract

A long standing problem in paleoceanography concerns the reconstruction of water temperature from δ^{18}O carbonate, which for freshwater influenced environments is hindered because the isotopic composition of the ambient water (related to salinity) affects the reconstructed temperature. In this paper we argue for the use of a non-linear multi-proxy method called Weight Determination by Manifold Regularization to develop a temperature reconstruction model that is less sensitive to salinity variations. The motivation for using this type of model is twofold: Firstly, observed nonlinear relations between specific proxies and water temperature motivate the use of nonlinear models. Secondly, the use of multi-proxy models enables salinity related variations of a given temperature proxy to be explained by salinity-related information carried by a separate proxy. Our findings confirm that Mg/Ca is a powerful paleothermometer and highlight that reconstruction performance based on this proxy is improved significantly by combining its information with the information of other trace elements in multi-proxy models. Using Mg/Ca, Sr/Ca, Ba/Ca and Pb/Ca the WDMR model enabled a temperature reconstruction with a root mean squared error of ±2.19°C for a salinity range between 15 and 32.

1 Introduction

To improve our understanding of global change and to assess human impact on various global warming, reconstructions of past temperatures are essential. Several natural archives record environmental information in their trace element and isotope proxy profiles (e.g., Freitas et al., 2009; Klein et al., 1996b; Epstein et al., 1953). Bivalve shells represent a suitable archive for reconstructing seasonal variations in ambient water conditions. Indeed, bivalves are sensitive to environmental conditions, have a global distribution, and are commonly found in archaeological sites (Pearce and Mann, 2006; Klunder et al., 2008; Butler et al., 2009). Bivalve shells thus offer the potential

for reconstructing seasonal variation of environmental conditions for a wide variety of environments, including fresh water systems (Versteegh, 2009), estuarine and marine environments from tropical (Aubert et al., 2009) to cold polar regions (Tada et al., 2006).

Many elemental and isotopic temperature proxies have been proposed and discussed (e.g., Klein et al., 1996a, 1996b; Epstein et al., 1953; Wanamaker et al., 2006). These and other studies reveal that though a given proxy may correlate well with an environmental parameter, the data usually show significant variation around the regression line, reflecting that the process of proxy-incorporation is much more complex than assumed originally (Wanamaker et al., 2007; Gillikin et al., 2005).

Most water temperature reconstructions based on biogenic carbonates are based on $\delta^{18}O$ records. For instance, for the common blue mussel (*Mytilus edulis*; the species studied in this paper) it has been shown that temperature reconstructions from shell $\delta^{18}O$ records can achieve excellent accuracy of 0.57 °C in Root Mean Squared Error (RMSE) (Wanamaker et al., 2007). However, this paleothermometer equation requires that the $\delta^{18}O$ value of the ambient water be known. This is obviously not possible for archeological specimens and given that the $\delta^{18}O$ value of the ambient water strongly depends on salinity (a salinity variation of 1 can incorrectly be interpreted as a change of 1 °C in water temperature), a proxy or model which is less sensitive to salinity variations may therefore significantly improve paleotemperature reconstructions (Faure, 1986).

Although several alternative (salinity-robust) temperature proxies have been proposed (e.g., Mg/Ca-ratios, Klein et al., 1996b; Sr/Ca ratios, Foster et al., 2009), most potential temperature proxies suffer from kinetic (Lorrain et al., 2005) and ontogenetic effects (Elliot et al., 2009). In the present paper we propose to combine several proxies into a multi-proxy model in order to counter such interferences. The multi-proxy model presented in this paper combines measurements of Mg/Ca and Sr/Ca ratios, known to be potential temperature proxies, with measurements of Ba/Ca ratios and Pb/Ca ratios which may help explain the kinetic and ontogenetic effects in the Mg/Ca and Sr/Ca signal.

1.1 Why multi-proxy models?

Two reasons can be invoked for promoting the use of multi- proxy models: (i) proxy signatures are likely influenced by several environmental factors and combining information carried by several proxies which are influenced by the same environmental conditions may help reduce variation; (ii) any further proxy which also is controlled by temperature, adds "temperature information" to the model.

The first and most important reason (i, above) is synthesized by the set of Eqs. (1), which express how a number of environmental parameters (e.g., temperature, salinity, chlorophyll concentration) all contribute to the final trace element signature of the archive. Solving this set of equations for the environmental parameters involves a new set of equations in which all environmental parameters can be described by multi-proxy equations, implying that all proxies add some information to the final paleo-temperature equation. For example: by combining an element that is mainly influenced by salinity with another element influenced by both temperature and salinity, it is possible to construct a model that is more robust across a range of salinities.

$$\left\{\begin{array}{l} \text{Mg} = a_1.\text{Temp} + b_1.\text{Sal} + d_1.\text{chl-}a + \ldots + C_1 \\ \text{Sr} = a_2.\text{Temp} + b_2.\text{Sal} + d_2.\text{chl-}a + \ldots + C_2 \\ \text{Ba} = a_3.\text{Temp} + b_3.\text{Sal} + d_3.\text{chl-}a + \ldots + C_3 \\ \ldots \end{array}\right\} \Leftrightarrow \left\{\begin{array}{l} \text{Temp} = \alpha_1.\text{Mg} + \beta_1.\text{Sr} + \varphi_1.\text{Ba} + \ldots + C_{1'} \\ \text{Sal} = \alpha_2.\text{Mg} + \beta_2.\text{Sr} + \varphi_2.\text{Ba} + \ldots + C_{2'} \\ \text{chl-}a = \alpha_3.\text{Mg} + \beta_3.\text{Sr} + \varphi_3.\text{Ba} + \ldots + C_{3'} \\ \ldots \end{array}\right\} \quad (1)$$

(ii) A second drive for using multi-proxy models is rather intuitive. Assuming that different proxies carry some temperature information it seems reasonable that a model based on the information of several proxies will yield more robust and accurate reconstructions, though this requires proper weighing for each proxy.

Despite these clear advantages, applications of multi-proxy models are scarce in the literature. Some steps in this direction are made by Klein et al. (1996b) and Schöne et al. (2006), though these authors rather use a secondary proxy to confirm a signal that is revealed by a primary proxy. Gentry et al. (2009) and Bice et al. (2006) discuss two approaches in which the influence of salinity on $\delta^{18}\text{O}_{\text{carbonate}}$ is eliminated by formulating

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an initial guess of the $\delta^{18}O_{water}$ using information from a secondary proxy. However, to the best of our knowledge multi-proxy models in which a given environmental parameter is described by a combination of several proxies have not been published yet, one exception being the work of Freitas et al. (2006) who demonstrate that a linear multiple regression analysis using Sr and Mg, significantly improves temperature estimates.

1.2 Why nonlinear multi-proxy models?

Considering that physiological processes within an archive building organism are nonlinearly influenced by environmental conditions such as e.g. temperature, plankton blooms (Cloern et al., 1995), optimal feeding temperature (Yukihira et al., 2000) the occurrence of nonlinear relationships between proxies and environmental conditions would not come as a surprise. Figure 2 shows an example of a substantially nonlinear relationship between bivalve shell proxies and water temperature (Vander Putten et al., 2000), highlighting a direct but complex influence of temperature on trace element uptake. However, such relationships have been traditionally described using linear equations (Klein et al., 1996b; Wanamaker et al., 2008), though some recent publications describe or advocate the use of inverse exponential (Clarke et al., 2009), exponential (Freitas et al., 2005) and even dynamical (Klunder et al., 2008) relationships.

Nonlinear relationships between proxies and environmental conditions are difficult to describe in a single mathematical equation but they can be modeled by several modern multivariate statistical techniques (Izenman, 2008). Most scientists are familiar with the classical linear multiple regression and dimensionality reduction methods, such as Principle Component Analysis (PCA), Cluster Analysis, etc. These methods, however, are developed to detect linear relationships and thus are not applicable to datasets that behave substantially nonlinear. To detect nonlinear relationships in a multi-dimensional space, recently developed multivariate statistical tools are needed (Izenman, 2008). The best known nonlinear multivariate statistical techniques in paleoclimatology are Artificial Neural Networks which are being used for reconstructing

ENSO events from coral records (Juillet-Leclerc et al., 2006) and in dendrochronology to reconstruct precipitation rates (Woodhouse, 1999) and temperature (Guiot et al., 2005). However, other techniques such as Support Vector Machines and Manifold Learning can be used for the same purpose (Bauwens et al., 2009).

Different nonlinear multivariate statistical techniques are thus available to analyze multidimensional datasets, but the choice of a specific technique will depend on characteristics of the dataset such as e.g., number of data, intrinsic variance, smoothness, periodicity. As a consequence, each dataset has its own "best method". Bauwens et al. (2009) compared three nonlinear multiple regression methods and concluded that manifold based methods were the most powerful tools for reconstructing paleo-environmental conditions based on proxy records in shells of short-lived bivalves. In the present paper we use the manifold based method: Weight Determination Manifold Regularization (WDMR) (Ohlsson et al., 2008, 2009) to build a salinity-robust model for reconstructing temperature using shells of the common blue mussel *Mytilus edulis*.

2 Data

2.1 Raw data

The trace element datasets used in this paper were originally published by Vander Putten et al. (2000) and Gillikin et al. (2006a,b). Both datasets consist of spatially well resolved measurements of Mg/Ca, Sr/Ca, Ba/Ca and Pb/Ca ratios along the shell's main growth axis for approximately two years old *M. edulis* specimens. For both studies laser ablation craters (from LA-ICP-MS analyses) were produced in the calcitic layer of the shell. The ablation craters were approximately 50 μm in diameter and were spaced every 250 μm. For each shell 45 to 65 ablations were performed over the shell section that grew during the period of monitoring. All specimens were sampled in the Scheldt Estuary (The Netherlands, Belgium); the exact geographical position of the four study sites is shown in Fig. 1.

The dataset of Gillikin et al. (2006a,b) consists of proxy records for a single shell sampled at the Knokke site that was monitored from February to September 2002.

Since the blue mussel stops growing when temperature drops below 8 °C (usually in autumn; Gillikin et al., 2009), the analyzed February to September period closely corresponds to a complete growth season. The data set of Vander Putten et al. (2000) concerns seven blue mussel shells from Terneuzen, four shells from Ossenisse and

5 four shells from Breskens (Figs. 1 and 3). These data cover the period from April to June 1996, which does not cover the full growth season of the blue mussel but includes spring, the period during which shell accretion is fastest and variations in trace element concentrations largest. The total dataset covers a salinity range from 15 to 31 and a temperature range from 6.8 °C to 18.6 °C for 1996 and from 8.7 °C to 19.3 °C for 2002.

10 ## 2.2 Data preprocessing

2.2.1 Linking proxy data to environmental information

The proxies were measured along the largest growth axis (i.e., along a distance scale) starting at the margin of the shell moving towards the umbo. Since temperature measurements are obtained on a time scale, linking proxy data to environmental information

15 is not straightforward. For both data sets the link between spatial and temporal scales was established using the anchor point-method (Paillard et al., 1996), implying that in between anchor points, growth is assumed linear. The anchor points for the Vander Putten et al. (2000) shells were a T_0 (marking on the shell), T_{final} (date of collection) and recognizable patterns in trace-elemental chemistry, such as a conspicuous Ba-

20 peak associated with the spring bloom. The anchor points for the Gillikin (2006a,b) dataset were obtained from pattern similarities between the $\delta^{18}O$ profile of shell carbonate and the water temperature profile monitored at the study site. The assumption of subsequent linear growth events, however, is an approximation since shell growth is variable (Schöne et al., 2005). Other methods to reconstruct the shell growth as

25 reviewed in de Brauwere et al. (2008) could not be applied to the datasets used in the present study, since these methods are designed for periodic signals and are not applicable to records covering only a single season, as is the case here.

2.2.2 Normalized data

Proxy signals in different specimens from the same species sampled at the same location are often similar but seldom identical. Since environmental variability is unlikely over the small spatial scale of a mussel bank, the variation can be seen as an intrinsic and unexplained variation we shall call "noise". Besides noise, site- and year- specific variation can occur. These variations due to differences in the environmental conditions are nevertheless informative. By normalizing the data the reconstructed environmental parameter will become dependent on the overall shape of the proxy record. Normalization was done by dividing the data by the standard deviation and subtracting the mean. This offers the advantage of the data becoming less sensitive to site and year specific variability as well as concentration shifts (see Fig. 3; and also Stecher et al., 1996; Gillikin et al., 2008) since these effects will be filtered out. The disadvantages, however, are that some potential useful information is lost and that temperature reconstructions are only possible when the proxy signal is measured over the full growth cycle.

2.2.3 Training and validation data

The data were divided into two parts: a training dataset consisting of 6 shells from the Terneuzen site in the Scheldt Estuary and a validation dataset consisting of shells from all 4 sites along the Scheldt Estuary, i.e., one shell from Knokke sampled in 2002, four shells from Breskens, one shell from Terneuzen and four shells from Ossenisse sampled in 1996 (Figs. 1 and 3). The fact that the specimen from Knokke is from a different year than the other shells provides the possibility to check whether the model is sensitive to year to year variability between proxies and environmental conditions. The training dataset was used to construct a model and the validation dataset to evaluate the computed model's performance.

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3   Methodology

3.1   The method: Weight Determination by Manifold Regularization (WDMR)

The mathematical details of the method called Weight Determination by Manifold Regularization (WDMR) are beyond the scope of the present paper and the interested
reader is referred to (Ohlsson et al., 2008, 2009). Interested users can also download a Matlab WDMR toolbox that is added as supplementary material to this paper, although we recommend contacting the corresponding authors to ensure correct use of the WDMR toolbox.

In the following we briefly describe the concept of the WDMR approach. Manifold
learning is an umbrella term for algorithms or methods for describing low-dimensional structures in data. A manifold can be defined as a low-dimensional structure which underlies a collection of high dimensional data, for example a curve in the space of Mg, Sr, Ba and Pb concentrations. An algorithm that builds on concepts from manifold learning is the nonlinear semi-supervised regression method called Weight Determination
by Manifold Regularization (WDMR) (Ohlsson et al., 2008). WDMR, like a manifold learning algorithm, finds descriptions of manifolds but unlike most manifold learning methods WDMR can utilize a training set for the description. If the temperature associated with a specific measurement of Mg, Sr, Ba and Pb in the training set is known, that information can be used in WDMR to impose a one-dimensional description of
the curve imitating the temperature. In the case that proxy composition are controlled solely by water temperature, concentrations of Mg, Sr, Ba and Pb would be restricted to a one-dimensional curve in the four-dimensional measurement space with each position on the curve having a temperature value associated with it. As a result the curve can be parameterized by the water temperature. The computed WDMR-model can
then be used to estimate the water temperature for any other dataset of Mg, Sr, Ba and Pb. As in all real-world problems there is of course noise associated to the measurements. And more importantly, the concentrations of Mg, Sr, Ba and Pb do not only depend on water temperature (they also depend e.g. on salinity and kinetics) and

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therefore the data will scatter around a one-dimensional curve. The assumption of a one-dimensional manifold is therefore only an approximation, but the performance of the computed model shows that this approximation is appropriate.

3.2 Comparing linear multiple regression to WDMR

To investigate the benefit of using nonlinear methods rather than linear methods we compared the reconstruction performance of models generated using WDMR with models obtained by classical linear multiple regression. Six shells from Terneuzen were used to train both the linear model and the WDMR model. The model performances were calculated for the four validation sets consisting of shells from the 4 study sites, including one additional shell from the training site (see Fig. 1). To calculate the model performance the Root Mean Squared Error (RMSE) between measured and reconstructed temperatures for each data point (i.e. each laser ablation crater) was used. The reconstructed temperatures for the nonlinear WDMR model and the linear multiple regression model were compared and the differences between their RMSE used to verify whether some proxy combinations benefited more than others from the nonlinear model.

3.3 Evaluation of proxy combinations

To investigate the benefit of a multi-proxy approach using the WDMR method and to examine the contribution of the different proxies, different models were constructed based on a limited number of proxies. In total 15 combinations of proxies were investigated. The RMSE values were used to quantify the model performances. For the nonlinear models seven unique contribution factors were defined per proxy in order to quantify the contribution of each proxy. These contribution factors are defined as the difference between the RMSE of the two models, run with different combinations of elemental ratios (Table 1). This allowed to evaluate how model performance changes as a result of including additional proxies. Increasing contribution factors reflect improved temperature reconstruction (Table 1).

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3.4 Salinity robustness test

All trace element combinations were tested for their robustness to salinity by using the different models to reconstruct the temperature based on the validation shells from the 4 sites along the estuarine salinity gradient.

4 Results

4.1 Comparing linear multiple regression to WDMR

Positive values of the RMSE differences between the linear and the WDRM approaches indicate the WDMR model to perform better. The nonlinear WDMR model results in a better reconstruction of the seasonal temperature pattern for the Knokke site, as shown in Fig. 4. Also for the tree other sites and for most proxy combinations the nonlinear WDMR model performs better than the linear multiple regression models in RMSE-sense (Fig. 5). This is true, in particular for the temperature reconstructions at Terneuzen and Knokke where only the Sr-only and the combined SrPb proxies do better with a linear model. The reconstruction performance of the nonlinear WDMR model is up to 1.5 ˚C better than the one for the linear model. Furthermore, the performance of nonlinear models is increasing when more proxies are included. This result confirms that relationships between a proxy and the controlling environmental condition can indeed be nonlinear. However, the weaker reconstruction performances of the nonlinear model for the Breskens and Ossenisse sites indicate that the nonlinear model over-fits the training data for some proxy combinations, such that in these cases linear models result in better reconstruction (Fig. 5). This is in particular true for Ba at the Breskens site, showing a distinct site-specific behavior which results in the linear model performing better.

4.2 Evaluation of proxy combinations and salinity robustness test

Figure 6 demonstrates that the four-proxy model generated with the WDMR method is relatively insensitive to changes in salinity, since the model is able to reconstruct the temperature for all study sites along the estuarine salinity gradient, without systematic

5 errors due to differences in salinity. The overall trend of reconstructed temperatures is very similar to the measured temperature, but the reconstructed temperature profiles show more variability. Though the best reconstruction is obtained for the validation shell from the same study site and collected at the same time as the training shells (RMSE = ±1.29 °C), the temperature reconstructions for the three other study sites are

10 still better than ±2.19 °C. The validation shell from Knokke, sampled in a different year than the training set, has a similar RMSE as the validation shells sampled in Ossenisse and Breskens, the same period as the training set. Therefore we can conclude that the model correctly resolves possible inter-annual variability in the proxies-temperature relationship.

15 The reconstruction performance of models trained for different proxy combinations is shown in Fig. 7. In general RMSE decreases with an increasing number of proxies. This trend is also observed in Table 1 where it is demonstrated that the use of an additional proxy in a multi-proxy model greatly improves reconstruction performance since most contribution factors (i.e., RMSE with proxy – RMSE without proxy) are positive.

20 The benefit of using a multi-proxy model is thus significant, although it is clear that not all proxies contribute equally to the final reconstruction and the four-proxy model is not necessarily the best model.

Table 1 shows that on average all proxies contribute positively to the final reconstruction. Mg can improve the RMSE of a temperature reconstruction with 0.72, on average.

25 Ba improves the RMSE of a temperature reconstruction with 0.42. Pb and Sr, however, show lower contribution factors of 0.20 and 0.04, respectively. The average contribution factors shown in Table 1 thus suggest that Mg and Ba contribute the most to an accurate temperature reconstruction. Ba, however, shows several negative contribution factors for the Breskens site, revealing site specific effects. However, information stored

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in the Sr-signature of the shell almost completely compensates for these site specific effects. This can clearly be seen by comparing the performance of the MgBa-model with the one of the MgSrBa-model in Fig. 7, with the latter yielding fairly accurate and salinity robust SST reconstructions. Adding Pb to this MgSrBa-model does slightly improve the reconstruction, although by not more than 0.2 °C.

5 Discussion

5.1 Comparing linear multiple regression to WDMR

Figure 4 makes it clear for the Knokke site that for most proxy combinations the nonlinear WDMR model results in more accurate temperature reconstructions than the linear multiple regressions. The reconstruction performance of the nonlinear model is up to 1.5 °C better than for the linear model. However, Fig. 5 also shows that some proxy combinations do not benefit from the nonlinear model. A linear model is less sensitive to model errors related to over-fitting. Temperature reconstructions from the Breskens shell, for instance, are improved when using a linear model based on proxy combinations containing Ba information. The site specificity of Ba that can be observed in Figs. 3 and 7 is discussed later in Sect. 5.3.2. Several relationships between proxy and environmental control factors reported in literature, behave linearly (Wanamaker et al., 2008; Carre et al., 2006) and in these cases a linear model with a lower number of parameters is still preferable. However, this should not be a reason for not using nonlinear methods since nonlinear methods can fit linear data, while nonlinear data cannot be described by linear regression methods.

5.2 Salinity robustness test

Using the WDMR-method to construct paleo-thermometer models yields accurate temperature reconstructions for shells from Terneuzen where the training set was sampled. This reconstruction shows that it is possible to reconstruct the temperature based on Mg, Sr, Ba and Pb. The reconstruction performance is slightly poorer for shells from

the other sites suggesting that the model is sensitive to site-specific variations. However, considering the salinity range from 32 (Knokke) to 15 (Ossenisse), the reconstruction performance (RMSE lower than 2.19 °C) for shells from a different site (and salinity) than the training set, is promising. Compared to other approaches for recon-
5 structing water temperature based on the blue mussel archive (Epstein et al., 1953; Wanamaker et al., 2006; Klein et al., 1996b) the performance of the method proposed here is of similar standard, if not better.

The multi-proxy model presented in this paper is built on four proxies of which two (Ba and Pb) were previously not considered to have potential as paleo-thermometers. It is
10 thus probable that this method will provide even better reconstructions when trained on a set of well known temperature sensitive proxies or when combined with another paleothermometry method (e.g., δ^{18}O, Epstein et al., 1953). Nevertheless, the use of nonlinear methods in general allows discovering less obvious (nonlinear) relationships between proxies and temperature. Consequently, it is possible that the use of mod-
15 ern nonlinear multivariate statistics (among which the WDMR method) will help to find new proxies with hidden paleothermometer potential. The use of nonlinear models in general will probably open new research paths in paleoclimatology.

5.3 Evaluation of proxy combinations

Figure 7 clearly shows that models based on a combination of proxies perform better
20 than single proxy models. But it is also clear that not all proxy combination perform as well. Table 1 gives an objective overview of the contributions of Mg/Ca, Ba/Ca, Sr/Ca and Pb/Ca to paleotemperature models. It thus appears that Mg, already known as a temperature proxy (Klein et al., 1996b; Wanamaker et al., 2006), shows the highest contribution to the temperature reconstruction. More surprising is that Ba and Pb,
25 which have not been proposed as temperature proxies, seem to contribute more to the temperature reconstruction than Sr which has been suggested as paleothermometer (Wanamaker et al., 2008).

5.3.1 Magnesium

The paleothermometer capacity of the Mg/Ca ratio is confirmed by our results. How-ever we can clearly see that the Mg-temperature relationship is not linear and there-fore nonlinear models do better. This nonlinear trend could reflect the fact that Mg incorporation in *M. edulis* is driven by a physiological temperature response with a maximal Mg incorporation around 16 °C (see Fig. 2). Except for the work of (Vander Putten et al., 2000), a similar Mg/Ca-temperature relationship showing maximal Mg uptake at an intermediate temperature, has not been reported in literature. Freitas et al. (2006) observe an exponential Mg-temperature relationship for different bivalve species. That relationship is similar to the abiogenic Mg/Ca-temperature relationship reported by (Oomori et al., 1987) and the temperature dependent Mg-incorporation in foraminifera reported by (Barker et al., 2005). Most published papers, however, pro-pose linear Mg-temperature relations for bivalves (e.g., Richardson et al., 2004; Pearce and Mann, 2006; Klein et al., 1996b, 1996a).

If this physiological temperature response is correct, it is very likely that metabolic processes affecting shell growth will interfere with Mg uptake. This would generate unexplained noise which can be considerably reduced by taking into account the infor-mation provided by other independent proxies. The nonlinear Mg-model, for example, reconstructs the temperature for the Knokke site with a RMSE of 2.75 °C (note that the Knokke shell is independent from the training set in time and space), while this error is reduced to 2.19 °C after including all four proxies in the model.

5.3.2 Barium

Except for the specimens from Breskens, the nonlinear Ba-model results in fairly good SST reconstructions, indicating that Ba uptake in the shell of *M. edulis* is partly driven by temperature. It is probable that the Ba-temperature relationship is indirect and rather reflects temperature driven plankton blooming or water mixing events (Lazareth et al., 2003; Barats et al., 2009). These indirect relationships can be informative but one

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should be aware of the additive noise or the model errors that could be created, possibly biasing the temperature reconstruction. Indeed bloom events are quite complex and are influenced by many environmental parameters such as river discharge, wind speed, insulation etc (Cloern et al., 1995). The failure of the Ba-model at the Breskens
site is probably due to this "additive noise and model errors". Indeed Fig. 3 shows that Breskens is the only site where a second Ba-peak is observed in spring, although the temperature profiles at the three study sites monitored in 1996 are very similar. Using Ba/Ca ratios as stand alone temperature proxy is thus not recommended. However, this does not mean than Ba/Ca ratios cannot add information into a multi-proxy
model. Several studies report that blooming events (induced by a larger food availability) can influence metabolism and induce variation in shell growth rate (Versteegh, 2009; Schöne et al., 2006; Gillikin et al., 2008).

5.3.3 Strontium

Contrasting with the studies that report a relation between Sr/Ca ratios and water
temperature in calcitic bivalve shells (Carre et al., 2006; Freitas et al., 2005; Wanamaker et al., 2008) our results indicate that Sr/Ca ratios do not carry much temperature information. The Sr/Ca-model computed in this paper does not result in satisfactory temperature reconstructions, neither for shells from the Terneuzen training site nor for the other sites. Moreover, when Sr is added to a multi-proxy model often a negative
impact is seen, indicating that Sr uptake is poorly influenced by temperature and also that the variations in Sr/Ca ratios do not contain significant information that assists in resolving the variation in other proxies. Nevertheless, Sr/Ca seems to have a positive influence on the site specificity of Ba/Ca, suggesting that Ba/Ca ratios and Sr/Ca ratios are influenced by a common environmental factor. Lazareth et al. (2003) also observed
some Sr/Ca maxima to coincidence with Ba/Ca-peaks. It is possible that the incorporation of both elements is influenced by shell growth rate as suggested at least for Sr/Ca by Carré et al. (2005), Gillikin et al. (2005) and Foster et al. (2009). Therefore, considering that Mg/Ca is a potential temperature proxy, even though it appears affected by

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variable shell growth rate and metabolic activity (Takesue et al., 2008), the combination of Mg/Ca with Sr/Ca and Ba/Ca can help explain a considerable fraction of the Mg/Ca signal noise. This is indeed observed in our dataset where the RMSE of the MgSrBa model is a significantly lower than the RMSE of the Mg/Ca model ($RMSE_{(MgSrBa\text{-}model)}$

5   $- RMSE_{(Mg\text{-}model)} = 1.28; 0.30; 0.40$ and 0.34 for Terneuzen, Breskens, Ossenisse and Knokke, respectively).

5.3.4   Lead

The Pb/Ca-model does not result in accurate temperature reconstructions (Fig. 4) and when adding Pb to a multi-proxy model, low or negative impacts are observed. This

10   means that Pb uptake is poorly influenced by temperature and also that the variation in Pb/Ca ratios do not contain much information helping to explain variation in other proxies. Nevertheless, when Pb/Ca is added to the MgBa model, contribution factors increase (Table 1). This suggests that Pb/Ca and Ba/Ca are influenced by a common parameter (possibly growth rate). However, there are no studies to confirm this hypoth-

15   esis and moreover, Pb/Ca ratios in shells have been shown to be strongly influenced by anthropogenic activities (Gillikin et al., 2005; Richardson, 2001) rather than natural climate related changes. So, we do not recommend including Pb in a multi-proxy model.

5.4   The use of the developed WDMR model

20   Several studies demonstrate that de incorporation of trace elements in bivalve shells is species specific (Gillikin et al., 2005) and site specific (Gillikin et al., 2006a). Moreover, some studies claim that trace elements are strongly influenced by diagenesis and thus not useful when studying archeological shell specimens (Ragland et al., 1979). Thus, the generic character of our model needs to be evaluated.

5.4.1 Species specificity

The model presented in this paper is trained on shells *M. edulis*. While we do not expect this model to be directly applicable to other species because Mg/Ca (the main player in the temperature reconstruction) is assumed to be driven by a physiological
5 temperature response which is probably species specific, a new WDMR model can be generated for other species not only including other bivalves but also corals, trees, sediments, etc. The WDRM method could be used to develop nonlinear models to reconstruct the paleoenvironment for all different types of natural climate achieves.

5.4.2 Year to year and site specific variations

10 The accurate temperature reconstruction for the shell from the Knokke site sampled during a different year than the training set indicates that the model could be used to reconstruct seawater temperature based on *M. edulis* shells sampled from the Scheldt Estuary and the North Sea. Year to year and site specific variations in trace element composition do not seem to affect the performance of the MgSrBa-model. Therefore
15 the model is probably accurate for a wider environment than studied here, although more tests are needed to exclude other site specific model errors similar to de Ba/Ca problem that is observed for the Breskens site.

 The problem of diagenesis is often mentioned in studies on trace elements in bivalve shells. Most studies on diagenetic effects on bivalve shells observe a general increase
20 or decrease of trace elemental ratios (Ragland et al., 1979). The WDMR method presented in this paper, however, uses normalized datasets which implies that the reconstructions are based on variations in the proxy signature rather than on proxy concentrations. It is thus likely that the WDMR model will be less sensitive to bias from diagenesis effects, compared to methods based on concentrations of proxies, but this
25 needs to be verified.

5.4.3 Building new models using the WDMR method

As mentioned before, the model presented in this paper is species specific, implying that a new model needs to be constructed for other species. Moreover, we believe the WDMR method could also be used to build a stronger model for *M. edulis* shells. The model presented in this paper is based on trace elements of which some were never linked to temperature before (i.e., Ba/Ca and Pb/Ca). Although Ba/Ca has clearly been shown to improve temperature reconstructions, a multi-proxy model that uses even more proxies with paleothermometry capacity would significantly improve the temperature reconstructions. Therefore, we encourage the construction of a WDMR model using high resolution measurements of Li/Ca ratios (Thebault et al., 2009), deuterium (Carroll et al., 2006) and oxygen isotopes (Epstein et al., 1953). On the other hand we also encourage exploring other elemental and isotopic measurements using the WDMR-method since this method is able to detect less evident relationships between a potential proxy and its environment.

The WDMR toolbox for Matlab is added as supplementary material to this paper, nevertheless we recommend contacting the authors to ensure the correct use of the WDMR toolbox.

6 Conclusions

6.1 The benefit of nonlinear methods

In this paper we show that using a nonlinear model to describe a proxy data set can improve temperature reconstruction performance with more than 1 °C compared to classical multiple regression techniques.

6.2 The benefit of combining proxies

Furthermore, we demonstrate that combining different proxies results in better temperature reconstructions. However, it is clear that not all proxies contribute equally to the final result. Our tests confirm that the Mg/Ca ratio in bivalve shells is a successful paleothermometer. We suggest that the Mg biomineralization is driven by a physiological response to changing temperature, which is possibly perturbed by metabolic activity and variable growth rate of the bivalve. The Combination of Mg, Ba and Sr into a multi-proxy model was successful because Ba and Sr reduce interfering effects due to metabolism and growth rate variation, thereby reducing the variance of the temperature prediction based on Mg.

6.3 The robustness of the WDMR method

The nonlinear multi-proxy model obtained by the WDMR is able to reconstruct temperature with a RMSE of less than 2.19 °C for a salinity ranging from 32 to 15. In comparison with other paleothermometry methods the performance using WDMR is good, if not better. This stresses that there is indeed a significant underlying low-dimensional structure in the proxy space. Although WDMR is a complex and sophisticated method, its success and robustness relies on its capability to nonlinearly combine proxy measurements into a multi-proxy model. One of the main messages of this contribution is therefore to encourage other researchers to combine their proxy measurements in one nonlinear multi-proxy model, since this will allow identifying new proxies with paleothermometer potential.

Supplementary material related to this article is available online at:
http://www.geosci-model-dev-discuss.net/3/1105/2010/
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Table 1. Seven unique contribution factors are defined per proxy. Every contribution factor is defined by the difference between the RMSE of a model based on a proxy combination whith the investigated proxy and the RMSE of a model based on a proxy combination without the investigated proxy. The average contribution of each proxy is given per study site and for the total validation set. Negative contribution factors are marked in red and mean that the corresponding proxy does not contribute to a better reconstruction.

	Terneuzen	Breskens	Ossenisse	Knokke	Average
Contribution of Mg					
RMSE using MgSr-RMSE using Sr	1.62	0.47	0.43	0.78	
RMSE using MgBa- RMSE using Ba	0.47	0.04	0.30	0.20	
RMSE using MgPb- RMSE using Pb	1.46	0.59	1.11	0.79	
RMSE using MgSrBa- RMSE using SrBa	1.13	1.03	0.20	0.28	
RMSE using MgSrPb- RMSE using SrPb	1.86	0.54	1.02	0.75	
RMSE using MgBaPb- RMSE using BaPb	1.06	0.70	0.17	0.31	
RMSE using MgSrBaPb- RMSE using SrBaPb	1.07	1.00	0.21	0.58	
Average	1.24	0.62	0.49	0.53	0.72
Contribution of Ba					
RMSE using MgBa- RMSE using Mg	0.62	−0.83	0.28	0.16	
RMSE using SrBa- RMSE using Sr	1.08	−0.21	0.81	0.94	
RMSE using BaPb- RMSE using Pb	0.70	−0.32	1.26	0.58	
RMSE using SrBaPb- RMSE using SrPb	0.93	−0.08	1.40	0.55	
RMSE using MgBaPb- RMSE using MgPb	0.31	−0.21	0.32	0.09	
RMSE using MgSrBa- RMSE using MgSr	0.59	0.35	0.58	0.44	
RMSE using MgSrBaPb- RMSE using MgSrPb	0.13	0.38	0.59	0.38	
Average	0.62	−0.13	0.75	0.45	0.42
Contribution of Sr					
RMSE using MgSr- RMSE using Mg	0.69	−0.05	−0.18	−0.10	
RMSE using SrBa- RMSE using Ba	0.00	0.13	0.23	0.10	
RMSE using SrPb- RMSE using Pb	−0.31	−0.07	−0.48	−0.09	
RMSE using MgSrPb- RMSE using MgPb	0.09	−0.12	−0.57	−0.13	
RMSE using MgSrBa- RMSE using MgBa	0.65	1.12	0.12	0.18	
RMSE using SrBaPb- RMSE using BaPb	−0.09	0.17	−0.34	−0.12	
RMSE using MgSrBaPb- RMSE using MgBaPb	−0.08	0.47	−0.30	0.15	
Average	0.14	0.23	−0.22	0.00	0.04
Contribution of Pb					
RMSE using MgPb- RMSE using Mg	0.97	0.16	0.42	0.26	
RMSE using SrPb- RMSE using Sr	0.13	0.3	−0.56	0.26	
RMSE using BaPb- RMSE using Ba	0.06	0.11	0.58	0.09	
RMSE using SrBaPb- RMSE using SrBa	−0.02	0.15	0.02	−0.13	
RMSE using MgBaPb- RMSE using MgBa	0.66	0.78	0.45	0.20	
RMSE using MgSrPb- RMSE using MgSr	0.37	0.10	0.02	0.23	
RMSE using MgSrBaPb- RMSE using MgSrBa	−0.08	0.12	0.03	0.17	
Average	0.30	0.21	0.14	0.15	0.20

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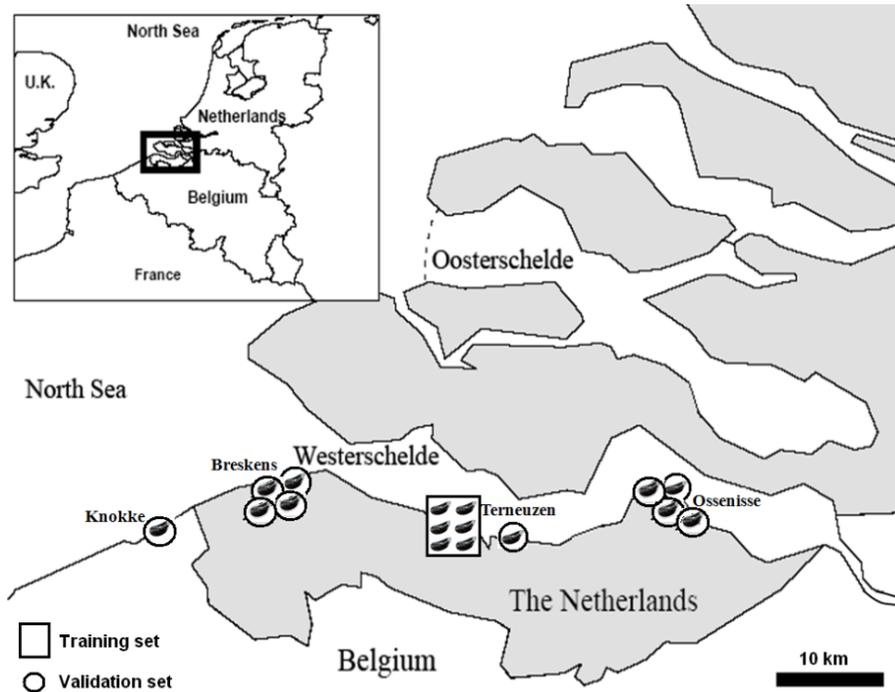
Fig. 1. Geographical position of the study sites in the Scheldt estuarine. Boxed: six shells from Terneuzen were used for training the models, Circled: the shells used for validation.

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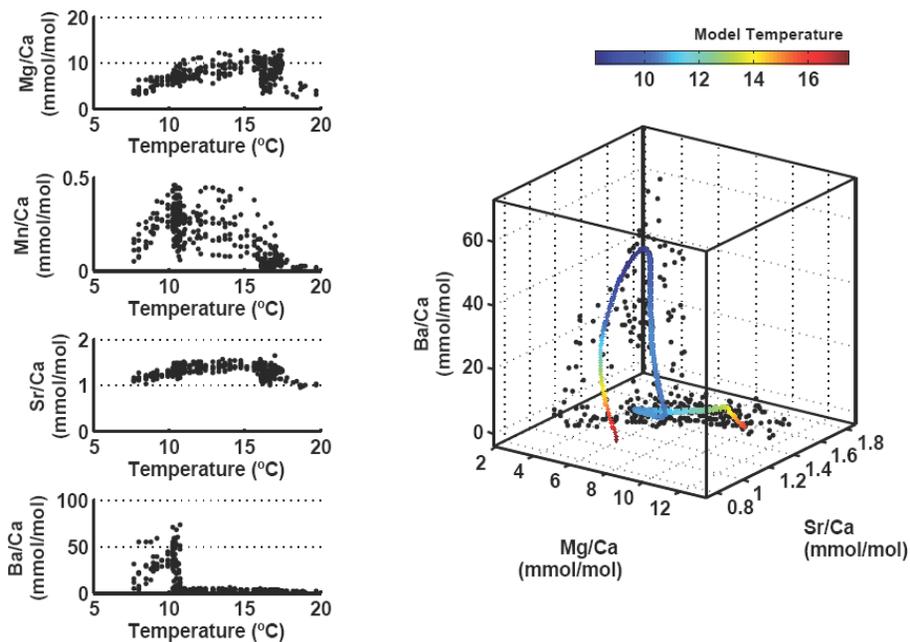
Fig. 2. Left: Ba/Ca, Sr/Ca, Mg/Ca and Pb/Ca ratios plotted against water temperature (Vander Putten et al., 2000). Right: Ba/Ca, Sr/Ca and Mg/Ca concentrations plotted against each other. The shown curve indicates how the concentrations are changing with water temperature.

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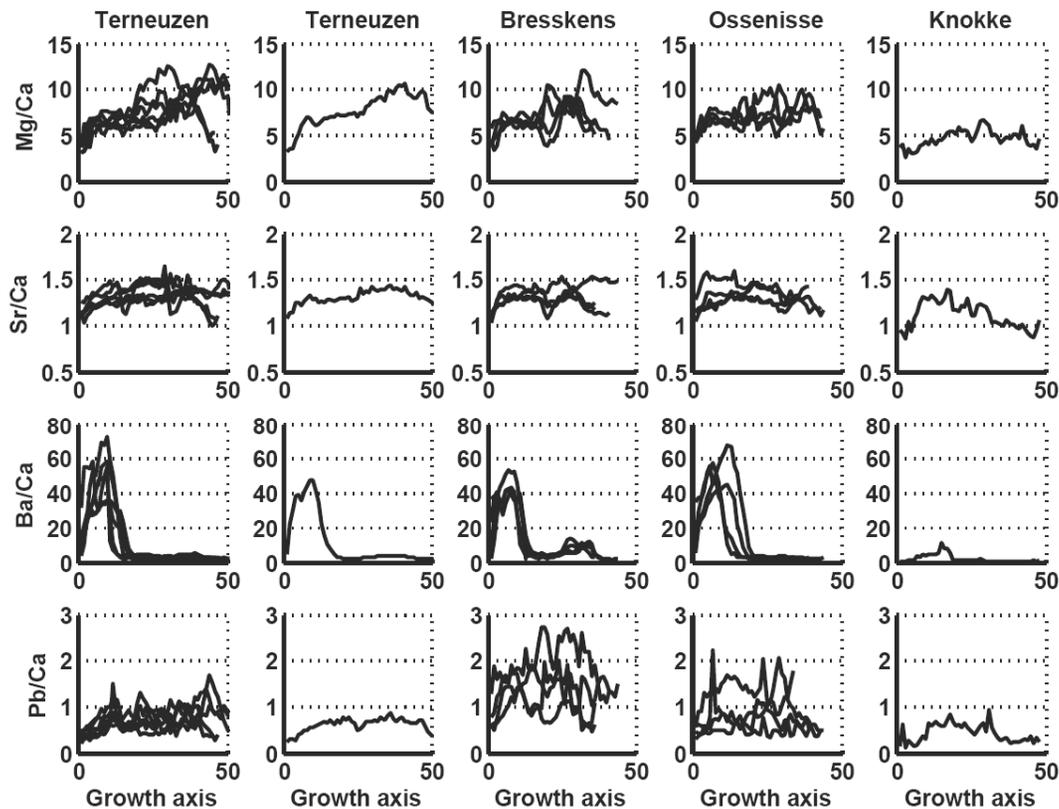
Fig. 3. Chemical signature along the growth axis of the shells used to train (first column) and to validate (columns 2–5) the models. The Trace element/Ca ratios are given in mmol/mol.
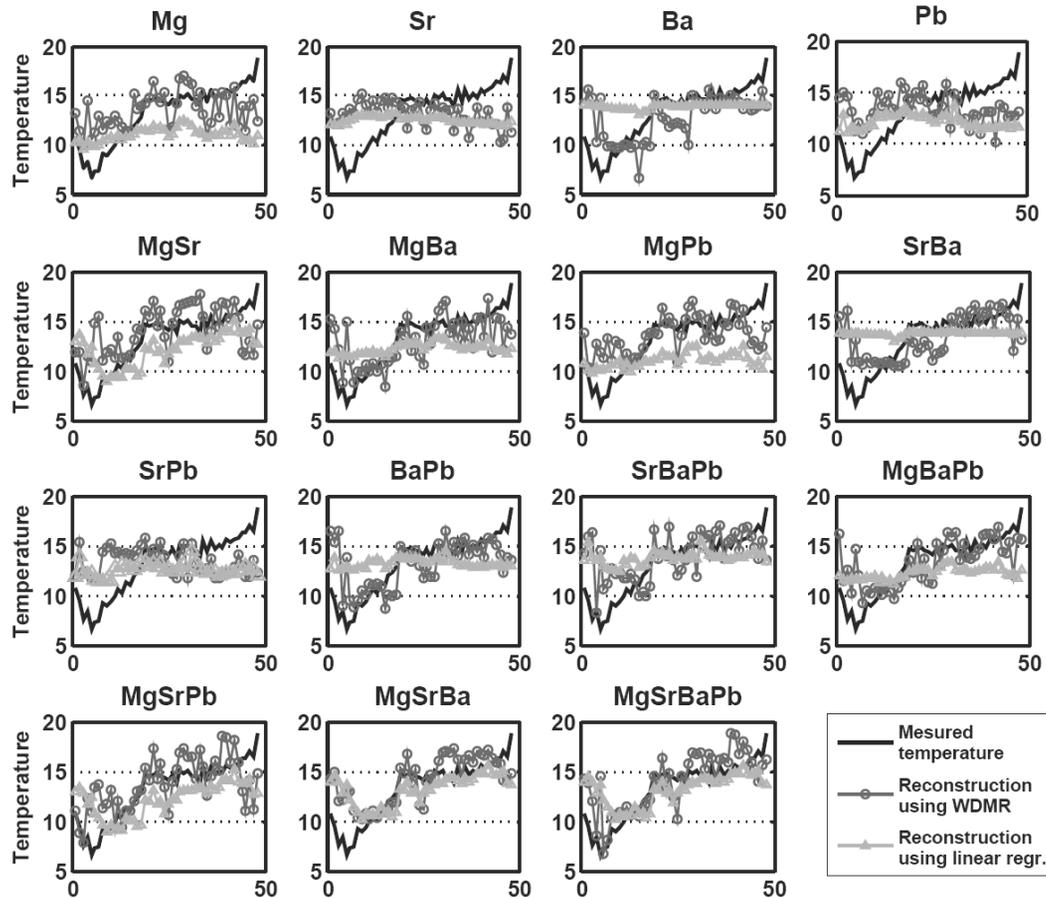
Fig. 4. Detailed visualization of the temperature reconstructions for the shell from the Knokke study site for all proxy combinations, the x-axis correspond with the sample numbers.
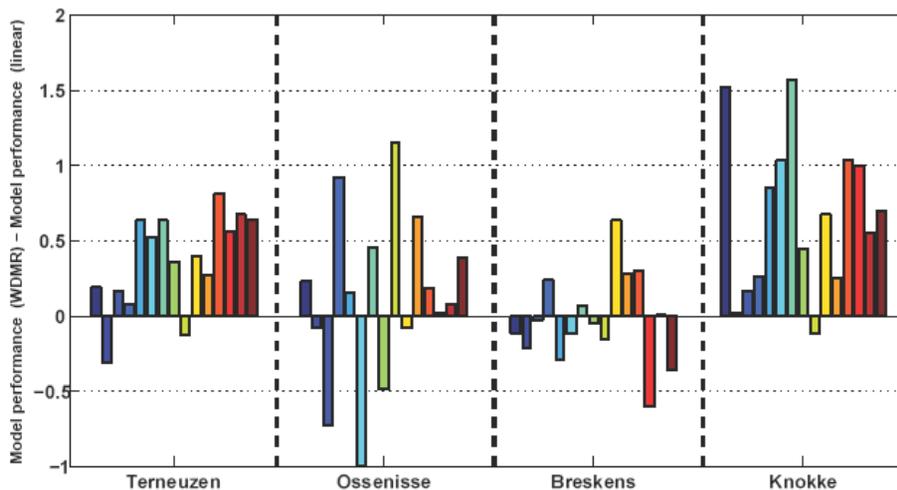
Fig. 5. The difference between the model reconstruction performance of the linear multi-proxy model (light grey stems) and non-linear multi-proxy model (dark grey bars). The models are trained on a training set of Terneuzen and tested 4 validation sets defined in Fig. 2.
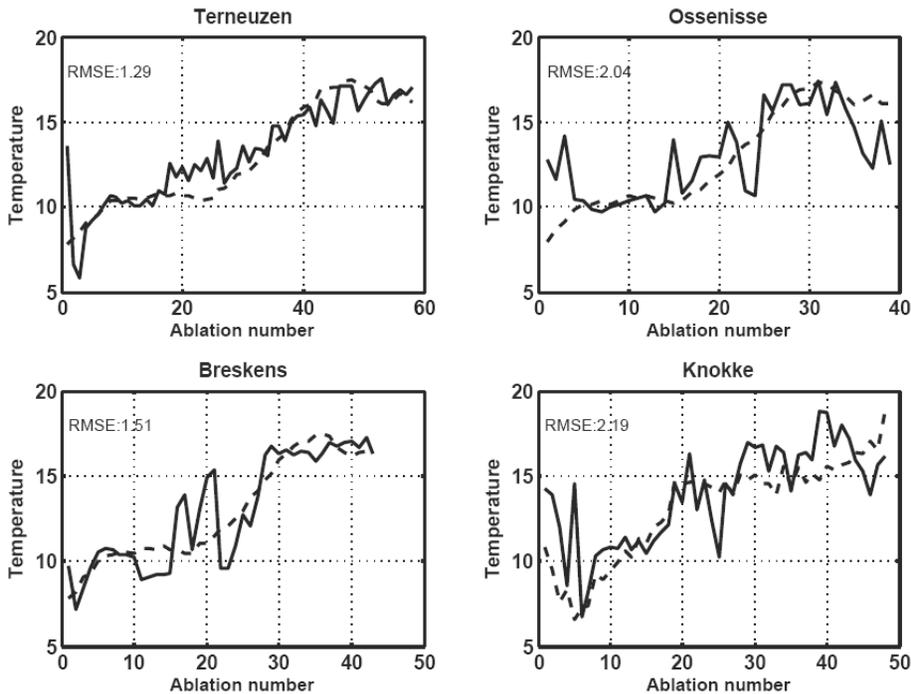
Fig. 6. Measured water temperature (dashed line) and reconstructed water temperature (solid line) obtained by the four-proxy WDMR model trained on the training set of Terneuzen and then tested on one validation shell from Terneuzen, Breskens, Ossenisse and Knokke.
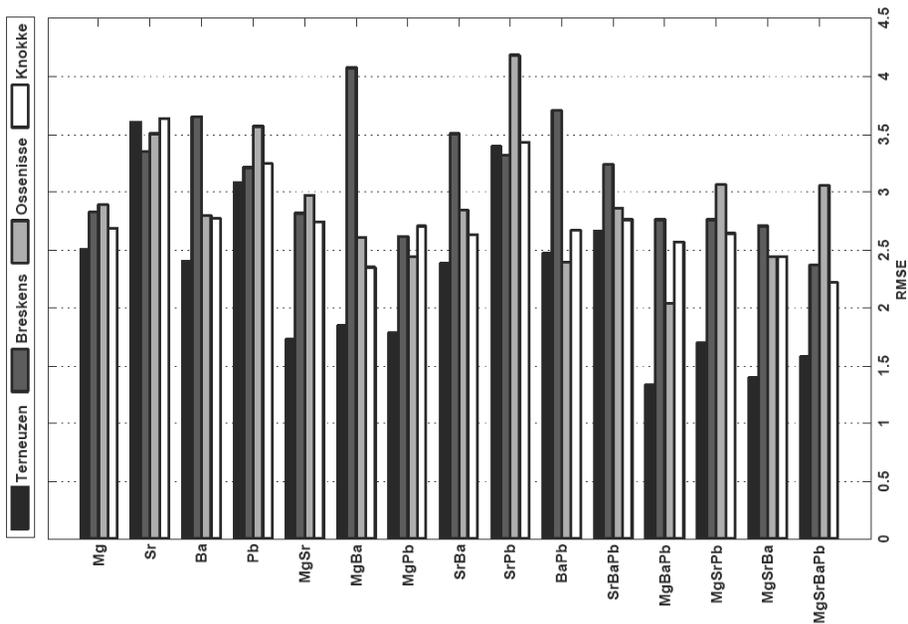
Fig. 7. Reconstruction performance of models in RMSE trained on training dataset with a limited number of proxies.