Geosci. Model Dev. Discuss., 3, C449–C456, 2010
www.geosci-model-dev-discuss.net/3/C449/2010/

**Geoscientific
Model Development
Discussions**

Interactive comment on "

A nonlinear multi-proxy model based on manifold learning to reconstruct water temperature from high resolution trace element profiles in biogenic carbonates" *by* M. Bauwens et al.

M. Bauwens et al.

msbauwen@vub.ac.be

Received and published: 14 October 2010

RESPONSE ON GENERAL COMMENTS

There is great confusion between the origins of the non-linearity, the incorporation of the trace elements, the role of the physical fractionation. This is revealed along the paper by multiple aspects. It could be judicious to explain first what a proxy is

and to examine the different steps making that a chemical measurement may be a relevant tracer. It is necessary to highlight how the non-linearity between the chemical measurement and the reconstructed parameter may be reflected. The reader needs to be prepared to the assumptions formulated in the conclusion, the possible role of the metabolism or/and growth rate. In the introduction it is never mentioned that the "proxy" (in this case trace element) is derived from biogenic material, which seems to me the main reason of the non-linearity of the signal. The authors could refer to: Weiner S. and Dove P. M. (2003) An overview of biomineralization. Process and the problem of the vital effect. In Reviews in Mineralogy and Geochemistry Volume 54 "Biomineralization" (eds. P. M. Dove, J. J. De Yoreo and S. Weiner). Mineralogical Society of America, pp. 1–29.

Thank you for this comment. I realized that I gave the wrong expectations about this paper by not mentioning clearly that de models presented are not based on a mechanistic understanding of the incorporation mechanisms of trace elements, or on the role of physical fractionation. Therefore I extended the introduction and the abstract to make the general statistical idea about the 'non-linear multi-proxy' more clear. I hope I now made clear that the reasons for using nonlinear multi-proxy models are purely statistical, although the results obtained by the statistical black-box models may reveal some more mechanistic understanding. I do understand that 'The reader needs to be prepared to the assumptions formulated in the conclusion' but detailing the proxy characteristics as well as the link between the proxies in the introduction, would give the reader the wrong impression that the proxies are 'selected' to be part of the model what is not the case. Therefore, the underlying proxy-incorporation processes are not described in the introduction, but discussed after presenting the results. In the discussion of "Section 5: Evaluation of proxy contributions" a more physiological interpretation is given to the contribution of every proxy in the multi-proxy model that is initially consider as a black-box model.

I added this sentence in the abstract:

“Although the models presented here are black-box models that do not use any prior knowledge about the proxies, the comparison of model reconstruction performances based on different proxy combinations do yield useful information about proxy characteristics.“

I added this sentence to the introduction:

“Such reconstructions are mostly based on the analysis of trace elements and isotopes in accreting biogenic or abiogenic substrates, called archives. The choice of the parameters (called proxies) to be analysed is based on prior knowledge of their relationship with an environmental variable as derived by observing such relationship in the present-day situation (Kucera et al., 2005).”

I extended the introduction with:

“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). However, proxies mostly appear influenced by several environmental parameters (e.g. Elliot et al. 2009, Foster et al. 2009). Moreover, the fact that these potential temperature proxies are recorded in biogenic material, makes them subject to physiology-related biases such as kinetic effects (Lorrain et al., 2005), methabolic effects (Strasser et al., 2008) and ontogenetic effects (Elliot et al., 2009). It becomes more and more clear that biomineralisation is a complex process, whose adequate study ideally requires the involvement of several disciplines (Weiner and Dove 2003).

In the present paper we investigate whether more complex, non-linear models are better suited for describing the integrated impact of environmental conditions, physiological state of the organism and a complex suit of biochemical and chemical processes, on proxy incorporation during bivalve shell growth. We propose to combine a suit of proxies, differentially influenced by environmental and biological controls, into a multi-proxy model. Multi-proxy models offer the advantage that variation in the different proxies yields information that is useful to resolve environmental and biological interferences.

The proposed multi-proxy model combines information on elemental ratios (in this case Mg/Ca, Sr/Ca, Ba/Ca and Pb/Ca) based on the two general (statistical) assumptions: (i) the proxies are influenced by the same environmental and intrinsic parameters, and therefore combining them may help explaining variation that was not understood before; (ii) the proxies are likely influenced to different degrees by temperature variation and, therefore, using temperature information derived from each of the proxies will yield more robust temperature reconstructions.

The models presented in this paper are not based on a mechanistic understanding of the incorporation mechanisms of the proxies. However, along this paper it becomes clear that the studied proxies do not contribute equally to the final temperature reconstructions. The contribution of each proxy was calculated, though, from the temperature reconstruction performances of different proxy combinations.”

RESPONSE ON SPECIFIC COMMENTS

p3-line22, you could argue that the "vital effect" term which is often used when the chemical response is not understood, necessitates a multi-proxies model.

I agree and added the following text to Section 1.1.:

“Though equations (1) as shown include only environmental parameters (Temp., Sal., Chlorophyll) it is clear that other, organism-related parameters such as shell growth, spawning events, metabolic activity, etc.... may be included as well. Such multi-proxy equations would resolve part of the ‘vital effect’ commonly invoked to explain a chemical response that is not understood. Note that solving a non-linear model with a large number of parameters is much more complex, but the idea behind it would be the same.”

p4-line8 – The most often applied multi-proxies are the couple _18O-Mg/Ca for the foraminifera and _18O-Sr/Ca for the corals, which implies the addition of the errors of the empirical calibrations used for isotopes and trace elements.

I am uncertain to what is meant with 'the addition of the errors of the empirical calibrations'. I guess the reviewer refers to the variance of measurement noise. The noise on a temperature reconstruction due to measurement noise will decrease with increasing number of proxies (in theory). The measurement noise is assumed to be independent and random for the different proxies. As such, an overestimation of the temperature by one proxy will be compensated by an underestimation of the temperature by another proxy, the more proxies are considered the more random noise will be removed.

p9-line3 – Salinity and kinetics are referred at the same level. It is not possible to compare salinity, an external forcing with kinetics, which is corresponding to the process of the mineral deposit. For example, temperature (an external forcing) may affect the proxy through kinetics. Incorporation of the trace elements or effects of growth rate are occasionally mentioned but the physical and/or chemical fractionation is never taken into account. About the choice of the multi proxy method well suited to non-linear system applied on the temperature reconstruction, it would be important to notice that temperature is the prominent factor acting on proxies, which determines the response to several tests.

I agree. Though it was not my intent to compare these two parameters, I cited these as being two independent factors influencing Sr/Ca ratio. I have reformulated the sentence as follows:

"And more importantly, it is unlikely that the concentrations of Mg, Sr, Ba and Pb will only depend on water temperature. Rather, they will depend also on other conditions such as salinity, food availability, shell growth or metabolism) and therefore the data will scatter around a one-dimensional curve in the Mg, Sr, Ba and Pb space."

p10 – It seems clear that there are three paragraphs: 1- comparison with multiple linear regression 2- evaluation of proxy combination 3- salinity robustness test why the proxy combination is mixed with the salinity test ?

I agree the structure was not logical. I restructured the text (as also suggested by

reviewer #2). In this new structure I combined the two paragraphs 'evaluation of proxy combination' and 'salinity robustness test' since evaluation of the proxies is strongly coupled to their robustness relative to salinity variations.

p13-line23 -It is true that Mg/Ca has not been so far identified as a SST proxy for bivalves but this proxy is commonly used for foraminifera. I was not clear. I did not say that Mg/Ca has not been so far identified as a SST proxy for bivalves. In contrast several studies confirm the paleothermometry capacity of Mg/Ca ratios for bivalves (e.g. Klein, Lohmann and Thayer 1996, Wanamaker et al. 2008). What I wanted to say at former p13-line23 is that only a few studies report an Mg-temperature relationship with a clear maximum.

I reformulated the sentences to clarify:

"Our results confirm the paleothermometry capacity of the Mg/Ca ratio as reported for several bivalve species by others (e.g. Klein et al., 1996b; Wanamaker et al., 2006). However, Figure 2 clearly shows that the Mg-temperature relationship is not linear. The Mg-temperature relationship seems to reflect that Mg incorporation in M. edulis is driven by a physiological response to temperature, with a maximal Mg incorporation around 16 °C."

p14-line3 - I do not see an explanation justifying the link between a physiological "optimal" temperature and the shell growth. Is it also an "optimal" temperature for growth rate?

I agree the paragraph was not clear. What I tried to say is that biological responses (physiology, metabolism, growth, food availability) are all closely coupled; therefore a proxy for shell growth and metabolic activity may explain some variations in a proxy that shows a physiological response.

I reformulated the paragraph:

"On the other hand, it has been shown that Mg/Ca ratios in shells are influenced by

growth rate (Ford et al., 2008) and by metabolic activity (Strasser et al., 2008). Moreover, Mg is shown to be incorporated majorly in shell organic matrix (Foster et al., 2008). Such biological controlls on Mg may explain why combining Mg with other proxies results in better reconstructions (see Figure 7). For instance if Mg incorporation in the shell indeed depends on physiology it is reasonable to assume that Mg incorporation will also be influenced by other vital factors, since the animal's physiological condition will be influenced by metabolic activity, growth rate, food availability and/or ontogenetic stage. Therefore, Sr (being a potential proxy for metabolic activity and growth rate), Ba (being a potential proxy for food availability) and Pb (also being influenced by ontogenetic stage) may explain some of the variation in the Mg/Ca profile of a shell."

p15-line9 – Could you develop the linkage existing between Sr/Ca and Ba/Ca?

Ba is a proxy of plankton blooms and thus 'food availability' (Thebault et al., 2009) which is likely to influence shell growth (for which Sr is a potential proxy). To clarify the text I added the following sentence to Section 5.3.2.: "Several studies report that phytoplankton bloom events can influence the metabolism of the filter feeding bivalve, thereby inducing variation in shell growth rate (Versteegh, 2009; Schöne et al., 2006; Gillikin et al., 2008). Therefore, it can be expected that the combination of Ba and Sr (a potential proxy for shell growth and metabolism) in a multi-proxy model will contribute to resolving variations in other proxies which are due to shell growth."

p15-line26 – Could you highlight the linkage existing between Pb/Ca and Ba/Ca, which could justify the assumption of a common parameter?

I don't think there is a clear link between Pb/Ca and Ba/Ca ratios. However, it has been observed that Pb/Ca ratios are influenced by temperature (Strasser, Mullineaux and Thorrold 2008) what would justify the combination of Pb/Ca with Mg/Ca. Moreover Pb/Ca profiles have been shown to show ontogenetic trends (Dick et al. 2007),

I added this sentence in Section 5.3.3. for clarification:

"A common forcing for Pb/Ca and Ba/Ca, however, has not been reported in literature. However, it has been shown that Pb incorporation in a bivalve shell is influenced by temperature (Strasser et. al., 2008) and Pb/Ca profiles sometimes show ontogenetic trends (Dick et al., 2007). These facts may explain the positive contribution factors of Pb in the multi-proxy models."

p16-line25 – Are you obliged to mention diagenesis which is another crucial question, but it does not add any new argument for the demonstration. I agree: I removed the paragraph.

The figure 5 does not provide strait forward information.

Thank you for this remark, I see that de legend of the future is missing and that the there are some errors in the figure caption. I changed the figure and the caption.

"Figure 5. Differences of model reconstruction performance obtained using the validation data between linear and non-linear multi-proxy models, for the 4 study sites. Positive differences indicate that the non-linear model performs better. The 15 different colors represent de 15 studied proxy combination.3

The figure 7 does not provide strait forward information.

I changed the caption:

"Model reconstruction performance expressed as RMSE for the four sites, as based on the Terneuzen training dataset using different proxy combinations."

Please also note the supplement to this comment:
http://www.geosci-model-dev-discuss.net/3/C449/2010/gmdd-3-C449-2010-supplement.pdf

Interactive comment on Geosci. Model Dev. Discuss., 3, 1105, 2010.