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Geoscientific Model Development Discussions

Interactive comment on "ShellTrace v1.0 – A new approach for modelling growth and trace element uptake in marine bivalve shells: Model verification on pacific oyster shells (Crassostrea gigas)" *by* Niels J. de Winter

Anonymous Referee #1

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De Winter presented a model for bivalves that can be used to compute the amount of shell material produced in specified time intervals including its average chemistry, weight, and relative proportion of the different microstructural types (foliated, chalky, prismatic). The model was tested with oysters. The author apparently used one valve per specimen, but did not say which one, the right or left.

The manuscript is very difficult to read and I had a hard time to understand for which purpose the model is really useful. L18-20: "This approach yields records of integrated total-shell trace element concentrations and accumulation rates, which shed light on

the rates and mechanisms by which these trace elements are incorporated into the shells of bivalves." I am honestly not sure how this can be accomplished by knowing the 3D bulk chemistry deposited in selected time slices. References are needed that demonstrate that such information is relevant. L413-417: "This study proposes a new method of modelling the growth, development [= ontogenetic development of shell shape?] and trace element incorporation in bivalve shell based on the location of growth increments in a cross section of the shell. The advent of a working model that can independently constrain growth and trace element uptake rates would greatly benefit the field of bivalve sclerochronology by providing independent control on shell growth rates, which influence the expression of geochemical proxies in the shell." No reference is provided for the relationship between growth rate and shell geochemistry. Shell growth patterns are a much better tool to determine growth rates than this model. Details are given further below (critique 1).

Sentence constructions are often very complicated and the phrasing is often not concise to the point. For example (L9-10): "However, many studies have shown that physiological changes related to growth of the bivalve may overprint these chemical tracers." Why not simply: ''Vital effects overprint chemical proxies of environmental change'. Or: L295-296 "Mapping and phase analysis in all shells resulted in a distinction between foliated calcite and chalky calcite layers in terms of chemical composition" Why not simply: 'Shell portions with foliated and chalky calcite differ chemically.'

More importantly, the author does not employ the standard terminology in sclerochronology, mineralogy and malacology. A few examples: The axis of maximum growth – along which the shells were cut – agrees approximately with the height axis of the shells, but not the length axis. The latter is defined as the distance from the posterior to the anterior margin. Shell width describes the broadest distance between the two valves. The author refers to growth lines (or bands) as increments (= the distance between consecutive growth lines). Foliated, prismatic and chalky refer to microstructures, not "mineral phases" (L321). The mineral phase of bivalve shells is $CaCO_3$ and occurs in various different polymorphs, depending on species and shell layer or shell portion, i.e., predominantly aragonite and calcite (not just calcite as stated in line 39), as well as vaterite and amorphous calcium carbonate etc.

Aside from that, the three biggest problems of the paper are (1) potential fields of application have not been properly described, (2) initial assumptions for the model are invalid and (3) the most relevant aspect of the model, chemistry and growth rate, have not been tested by independent means.

As for critique 1 – potential fields of application. There may be interest to know how carbonate production rates and biomass changed through time, and how much CO2 was sequestered by bivalves and other organisms. This could be accomplished by the analysis of shell volumes produced in specified time intervals. However, de Winter placed paleoclimate research and bivalve sclerchronology in the foreground without actually detailing how precisely these fields can benefit from his model. For example, the chemistry in a specified volume of a microstructurally and thus, chemically highly heterogeneous shell is – in my view – of limited relevance for paleoclimate research. The formation of different microstructures may be environmentally controlled, but are also governed by biomechanical needs. Since the different microstructures vary chemically (also mentioned in the ms, but no citations provided), chemical analyses should be limited to the same shell layer and microstructure. The author needs to explain and support by references why he thinks that the chemistry of a contemporaneously formed shell volume is relevant.

To assign dates to a shell, to determine how much shell material was deposited each day (L14) or month, the shell growth patterns can be consulted (note, no "proxy" is needed to "estimate age": L281). In fact, daily growth lines have been reported from this species (e.g., Barbin et al. 2008 DOI 10.1007/s00531-006-0160-0) and could have been used to determine the duration of the growing season and assign (calendar) dates to any portion of the shell. It is relevant to point out that no bivalve grows uninterruptedly through the year, because otherwise no growth lines (= reflecting periods of

retarded and ceased growth) would have been developed! One will certainly find less than 365.25 daily increments in an annual growth increment of a modern shell. In addition, the width of these daily increments provides information on the seasonal rate of shell formation which most certainly differs from the seasonally resolved growth curves shown in Figure 5 (upper left). Unfortunately, de Winter based his age model only on annual growth patterns and regular oscillations in some element curves (L331), which he interpreted as seasonal ("periodic": L306) variations. I wish to point out that there is still no consensus on the use of trace and minor elements in bivalves as environmental proxies, and I was unable to find any evidence in the manuscript supporting the assertion that the element levels in the studied specimens were actually controlled by the environment. The Van Bertalanffy curve may be able to approximate the cumulative annual shell growth, but the portions between the points in Figure 5 should not be overinterpreted and used to obtain a "daily" (L14) resolved shell growth record. Interestingly, the term "daily" is only used in the Abstract, but nowhere else in the manuscript. Instead, the author used the term "sub-annual" (L423) and also introduced the term "sub-increments" without explaining what this actually means. Is this referring to the differences in brightness resulting from the foliated and chalky microstructures?

As for 2 – false initial assumptions. I agree that a model approximates the real world, but may not perfectly resemble it. One may accept for a moment that the model reconstructed mass and volume with an error of 21%, which is attributed to variable shell thickness, specifically toward the posterior and anterior margins, possible ontogenetic changes in microstructure, organic content and porosity etc. But what also varies toward the anterior and posterior sides is the shell chemistry (e.g., Carriker et al 1991 Marine Biology 109, 287-297), and I dare to predict that the microstructure (including the relative proportion of foliated, prismatic and chalky microstructures etc.) varies in these directions as well, and with it does the chemistry (and the density). Interpolating the chemistry in a volume of contemporaneously precipitated shell portion from a single (2D) cross-section is therefore not valid; the chemical and structural heterogeneity is too large and cannot be modeled as presented.

As for 3 – model not tested. The paper would gain more strength if the model outcome was tested (not just mass and weight). In particular, daily growth patterns in the cross-section could have been used to test how well the Van Berlalanffy curve estimated varying seasonal growth rates. To test how well the volume of shell (deposited in selected time intervals) was estimated, the shells should be cut in various different angles. Computer tomography would provide even more reliable volumetric data and may also give information on spatial changes of the shell microstructure. In addition, the chemistry must be tested in different portions of the shells, particularly toward the posterior and anterior ends. And if the application in paleoclimate research stays in the foreground, then the 3D chemical data must be compared to instrumental environmental records. This certainly also requires a robust temporal alignment of the shell record which daily growth pattern analysis can provide.

In conclusion, the paper needs rigorous rewriting and refocusing. Standard terminology must be adhered to. A native speaker must read the ms.

Selected other issues, more provided in annotated pdf: In various places I missed proper references. For example, L65+66: "All these physiological changes, such as variations in growth and metabolic rate, shell mineralogy and spawning events, which affect the incorporation of trace elements into the shell of bivalves, complicate the use of trace element records to complement environmental reconstruction by stable isotope sclerochronology, (Klein et al., 1996b; Gillikin et al., 2005; Immenhauser et al., 2005; Freitas et al., 2006)." None of the cited articles refer to spawning-controlled element load.

L77: Paper "under review" cannot be cited.

L116-118: "Errors of reproducibility of μXRF measurements are generally higher than the instrumental error and depend on the integration time and the excitation energy of the element (see de Winter and Claeys, 2017; de Winter et al., 2017)." Is there really no reference predating 2017 that arrived at the same conclusion?

L122-123: "Timing of shell deposition was inferred from annual cyclicity in trace element profiles." [cyclicality!] No reference provided for this assertion.

L95/96: Shells were "sectioned longitudinally along their axis of maximum growth using a slow rotating, diamond coated saw".

Reference list is done sloppy. Genus and species must be italicized. In "δ18O" 18 must be superscript. Nouns in journal names must be capitalized.

Figure 2: Meaning of colors in XRF scan?

Figure 4: Size of letters varies too much (scales and axes' numbers). Why are annual growth lines not contouring the microstructure (compare e.g., Mouchi et al doi:10.1007/s00227-016-3040-6). Why are some years in enlarged hinge image flipped by 180°? Use "μ" not "u". Scale bars are far too thick. X-axis of graph must be mirrored (most recent year must be to the right, time axis should have same orientation as shell in topmost figure. Error bars missing.

Figure 6: Purpose of plotting 2D shell again? You are showing 3D chemical data... Numbers on axes are far too small. Green is not legible. Do not use colors for axes' labels. Where are the error bars?

Please also note the supplement to this comment:
https://www.geosci-model-dev-discuss.net/gmd-2017-137/gmd-2017-137-RC1-supplement.pdf

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