



# Quantification and propagation of errors when converting vertebrate biomineral oxygen isotope data to temperature for palaeoclimate reconstruction



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## ARTICLE INFO

### Article history:

Received 4 March 2014

Received in revised form 3 July 2014

Accepted 6 July 2014

Available online 18 July 2014

### Keywords:

Phosphate

Enamel

Regression

Calibration

Temperature

Palaeoclimate

## ABSTRACT

Oxygen isotope analysis of bioapatite in vertebrate remains (bones and teeth) is commonly used to address questions on palaeoclimate from the Eocene to the recent past. Researchers currently use a range of methods to calibrate their data, enabling the isotopic composition of precipitation and the air temperature to be estimated. In some situations the regression method used can significantly affect the resulting palaeoclimatic interpretations. Furthermore, to understand the uncertainties in the results, it is necessary to quantify the errors involved in calibration. Studies in which isotopic data are converted rarely address these points, and a better understanding of the calibration process is needed. This paper compares regression methods employed in recent publications to calibrate isotopic data for palaeoclimatic interpretation and determines that least-squares regression inverted to  $x = (y - b) / a$  is the most appropriate method to use for calibrating causal isotopic relationships. We also identify the main sources of error introduced at each conversion stage, and investigate ways to minimise this error. We demonstrate that larger sample sizes substantially reduce the uncertainties inherent within the calibration process: typical uncertainty in temperature inferred from a single sample is at least  $\pm 4$  °C, which multiple samples can reduce to  $\pm 1$ – $2$  °C. Moreover, the gain even from one to four samples is greater than the gain from any further increases. We also show that when converting  $\delta^{18}\text{O}_{\text{precipitation}}$  to temperature, use of annually averaged data can give significantly less uncertainty in inferred temperatures than use of monthly rainfall data. Equations and an online spreadsheet for the quantification of errors are provided for general use, and could be extended to contexts beyond the specific application of this paper.

Palaeotemperature estimation from isotopic data can be highly informative for our understanding of past climates and their impact on humans and animals. However, for such estimates to be useful, there must be confidence in their accuracy, and this includes an assessment of calibration error. We give a series of recommendations for assessing uncertainty when making calibrations of  $\delta^{18}\text{O}_{\text{bioapatite}} - \delta^{18}\text{O}_{\text{precipitation}} - \text{Temperature}$ . Use of these guidelines will provide a more solid foundation for palaeoclimate inferences made from vertebrate isotopic data.

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## 1. Introduction

Oxygen isotope analysis of bioapatite in vertebrate remains (bones and teeth) and shell carbonates in terrestrial and marine invertebrates are commonly used to address questions on palaeoclimate, palaeoecology and palaeotemperature from the Eocene to the recent past (e.g. Lécolle, 1985; Fricke et al., 1995; Zanchetta et al., 2005; Zanazzi et al., 2007; Van Dam and Reichart, 2009). It is sometimes possible to

use  $\delta^{18}\text{O}_{\text{bioapatite}}$  values to address the questions of interest directly, without requiring the data to be converted/calibrated to other forms (e.g. Forbes et al., 2010; Hallin et al., 2012). In many isotopic studies, however, the data are converted to quantitative estimates of the oxygen isotopic value of precipitation and thence to temperature (Navarro et al., 2004; Tütken et al., 2007; Arppe and Karhu, 2010; Skrzypek et al., 2011). These investigations require two data conversions that are based on well demonstrated correlations:

Z1 A species-specific conversion, using  $\delta^{18}\text{O}_{\text{bioapatite}}$  to estimate the mean isotopic composition of ingested water ( $\delta^{18}\text{O}_{\text{drinking water}}$ ) (Longinelli, 1984; Luz et al., 1984; Luz and Kolodny, 1985; Kohn, 1996). For the purposes of palaeoclimatic reconstruction

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$\delta^{18}\text{O}_{\text{drinking water}}$  is typically assumed to be equivalent to local mean  $\delta^{18}\text{O}_{\text{precipitation}}$ ;

- Z2 A regionally-specific conversion, using the estimated value of mean  $\delta^{18}\text{O}_{\text{precipitation}}$  to estimate mean air temperature  $T$  (Rozanski et al., 1992), which relates to the period the bioapatite was growing.

These correlations exist because of physical laws that govern the movement of isotopes through the biological and hydrological systems, and they remain consistently statistically significant across geographical regions and species (Dansgaard, 1964; Longinelli, 1984).

Defining accurate empirical mathematical relationships between these variables is complicated both by the problems in obtaining reliable primary data and by the effect of other variables that introduce uncertainties into the relationships themselves (Kohn and Welker, 2005). These uncertainties originate from many parameters, comprising biological (including species effects, population variability, variability in use of different water sources), environmental (such as latitudinal effects, rain variability, isotopic variation between potential water sources) and analytical (preparation techniques and measurement uncertainty) effects.

Published equations between temperature and the oxygen isotopic values of bioapatite and precipitation (henceforth referred to as  $\delta^{18}\text{O}_{\text{bioapatite}} - \delta^{18}\text{O}_{\text{precipitation}} - T$ ) are developed using regression analyses to obtain lines of best fit in the form  $y(x) = ax + b$  (Table 1). These may be used to calibrate data if the correlation is strong enough (Lucy et al., 2008). Recent examples from the literature make clear, however, that different mathematical practices are currently employed for undertaking the regression, and we will argue that not all methods are equally appropriate.

The spread of the data about a line of best fit represents the combined effect of all the sources of uncertainty. We show that when a best-fit correlation is used to convert new isotopic measurements, this spread makes an important contribution to the resultant uncertainty, and it must be taken into account, even if the line of best fit appears well constrained. If all the uncertainties are acknowledged, then the calibrations can be a useful method for generating first-order estimates of variables of interest in palaeoclimatic research. We will demonstrate that the uncertainties in the empirically-derived isotopic relationships, and the natural variability of new samples about those relationships, lead unavoidably to significant uncertainty in estimates of  $\delta^{18}\text{O}_{\text{precipitation}}$  and temperature. Moreover, the calibrations require several steps of data conversion, and the uncertainties need to be combined appropriately. Whilst some researchers give some information

about uncertainties in individual correlations (Grimes et al., 2003; Bernard et al., 2009; Van Dam and Reichart, 2009; Pollard et al., 2011; Stevens et al., 2011; Pryor et al., 2013), others do not explicitly quantify the statistical uncertainties inherent in their calculations (Ukkonen et al., 2007; Iacumin et al., 2010).

Here, we explore the application of standard statistical analysis to the issue of data calibration in the context of generating estimates of past temperature across a wide span of geological time (Delgado Huertas et al., 1995; Tütken et al., 2007; Ukkonen et al., 2007; Van Dam and Reichart, 2009; Arppe and Karhu, 2010; Krzemińska et al., 2010; Matson and Fox, 2010; Fabre et al., 2011; Skrzypek et al., 2011; Kovács et al., 2012). Our methods are similar to those used in Pollard et al. (2011) who outline the errors associated with inferring geographical origin from individual human bioapatite measurements. We first review some of the methods commonly used for regression analyses that facilitate the conversion of  $\delta^{18}\text{O}_{\text{bioapatite}} - \delta^{18}\text{O}_{\text{precipitation}} - T$ . A regression technique is then established that is statistically valid and appropriate for the datasets being employed, and the reasons for choosing this method are explained in detail. A method for calculating the uncertainties involved in the data calibrations is then presented, introducing the underlying mathematical model and the formulae which comprise the basis of the calculation. A digital spreadsheet that researchers may download and use to process their own data is also presented (Supplementary data). We then use our model to demonstrate some trends that arise from error calculations and conclude with a series of recommendations concerning the handling of errors when making  $\delta^{18}\text{O}_{\text{bioapatite}} - \delta^{18}\text{O}_{\text{precipitation}} - T$  conversions. The primary calibration equations discussed in this paper focus on the conversion relationships developed for horse (Delgado Huertas et al., 1995) and elephants (Ayliffe et al., 1992); although based on small datasets, both are widely applied (Delgado Huertas et al., 1995; Bos et al., 2001; Tütken et al., 2007; Ukkonen et al., 2007; Arppe and Karhu, 2010; Krzemińska et al., 2010; Matson and Fox, 2010; Fabre et al., 2011; Skrzypek et al., 2011; Kovács et al., 2012). We use them as an example to show that correct mathematical handling of the data facilitates a more rigorous data-conversion process, and gives a clearer statement of the inherent uncertainties in the predictions being made from the existing data.

## 2. Data conversion on enamel carbonates

By convention, the calibration equations of interest (e.g. for Z1) are typically expressed in terms of  $\delta^{18}\text{O}_{\text{bioapatite}}$  values measured on the phosphate moiety in the bioapatite structure, quoted relative to the SMOW/VSMOW isotopic standards. Enamel carbonates offer an

**Table 1**

Examples of equations that can be used for calibrating  $\delta^{18}\text{O}_{\text{enamel}}$  data in palaeoclimatic and palaeoecological investigations. The right-hand columns give values of parameters calculated using the methodology outlined in this paper.

Conversion	Equation (as published)	$r^2$	Reference					
A1								
PDB → SMOW	$\delta^{18}\text{O}_{\text{VSMOW}} = 1.03091 \delta^{18}\text{O}_{\text{PDB}} + 30.91$	1.00	Coplen et al. (1983)					
A2				$n$				
Carbonate → phosphate	$\delta^{18}\text{O}_{\text{phosphate}} = 0.98 \delta^{18}\text{O}_{\text{carbonate}} - 8.5$	0.98	Iacumin et al. (1996)	17				
Z1 (species specific)				$n$	$\bar{x}$	$S_{y/x}$	$\delta a$	$\delta \bar{b}$
Mammoth	$\delta^{18}\text{O}_{\text{enamel}} = 0.94 (\pm 0.10) \delta^{18}\text{O}_{\text{precipitation}} + 23.3 (\pm 0.7)$	0.85	Ayliffe et al. (1992)	17	-5.4	1.33	0.101	0.324
Horse	$\delta^{18}\text{O}_{\text{enamel}} = 0.71 \delta^{18}\text{O}_{\text{precipitation}} + 22.6$	0.77	Delgado Huertas et al. (1995)	23	-5.8	1.71	0.084	0.357
Z2 (regionally specific)				$n$	$\bar{T}$	$S_{x/T}$	$\delta a_T$	$\delta \bar{b}_T$
Europe <sup>a</sup>	$\delta^{18}\text{O}_{\text{precipitation}} = 0.59T_{\text{mean}} - 14.24$	0.54	Rozanski et al. (1992)	47				
Europe <sup>b</sup>	$\delta^{18}\text{O}_{\text{precipitation}} = 0.53T_{\text{mean}} - 13.74$	0.60	This study	34	9.9	0.92	0.076	0.16
Kraków (annual data) <sup>c</sup>	$\delta^{18}\text{O}_{\text{precipitation}} = 0.57T_{\text{mean}} - 14.50$	0.36	This study	28	8.2	0.67	0.149	0.13
Kraków (monthly data) <sup>c</sup>	$\delta^{18}\text{O}_{\text{precipitation}} = 0.32T_{\text{mean}} - 12.54$	0.59	This study	334	8.2	2.10	0.015	0.11
Vienna (annual data) <sup>d</sup>	$\delta^{18}\text{O}_{\text{precipitation}} = 0.65T_{\text{mean}} - 16.37$	0.28	This study	45	10.2	0.83	0.158	0.12
Vienna (monthly data) <sup>d</sup>	$\delta^{18}\text{O}_{\text{precipitation}} = 0.39T_{\text{mean}} - 13.70$	0.60	This study	516	10.3	2.37	0.014	0.10

<sup>a</sup> Full dataset unavailable for analysis; equation taken from Fig. 4A in Rozanski et al. (1992).

<sup>b</sup> General European relationship defined using 34 European monitoring stations in the Global Network of Isotopes in Precipitation (GNIP)/WISER online database under 500 m altitude that had more than five complete years of data (Supplementary data).

<sup>c</sup> Equations defined using data downloaded from the WISER database (1975–2002).

<sup>d</sup> Equations defined using data downloaded from the WISER database (1961–2005).

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