COMPOSITIONAL DATA ANALYSIS IN ARCHAEOMETRY

M.J. Baxter[1], **C.C. Beardah**[1], **H.E.M. Cool**[2]**and C.M. Jackson**[3]
[1]School of Science, Nottingham Trent University, UK; *michael.baxter@ntu.ac.uk*
[2]Barbican Research Associates, 16 Lady Bay Road, West Bridgford, Nottingham NG2 5BJ, UK
[3]Department of Archaeology, University of Sheffield, Northgate House, West Street, Sheffield S1 4ET, UK

1 Introduction

We shall call an $n \times p$ data matrix fully-compositional if the rows sum to a constant, and sub-compositional if the variables are a subset of a fully-compositional data set[1]. Such data occur widely in archaeometry, where it is common to determine the chemical composition of ceramic, glass, metal or other artefacts using techniques such as neutron activation analysis (NAA), inductively coupled plasma spectroscopy (ICPS), X-ray fluorescence analysis (XRF) etc. Interest often centres on whether there are distinct chemical groups within the data and whether, for example, these can be associated with different origins or manufacturing technologies.

Strictly speaking such data are always sub-compositional since only a subset, typically up to about 30, of the 91 naturally occurring elements are measured. In practice, if all the major components of a composition are measured, data may be approximately fully-compositional. We shall distinguish here between major and minor oxides, measured as a percentage, and trace elements measured in parts per million and usually present at levels of less than 0.01%. In the analysis of archaeological glass it is quite common to determine 10–11 major and minor oxides, excluding silica (SiO_2) the main component, and then determine silica, approximately, as the difference of their sum from 100%. In the analysis of ceramics, trace element data are widely used, sometimes exclusively so.

Since the mid-1970s it has been common to analyze such data using multivariate methods of which cluster analysis and principal component analysis (PCA) are the most common. Usually data are either standardized or, following the influential paper of Bieber and others (1976), logarithmically transformed to base 10 without subsequent standardization. Proponents of the log-ratio approach to compositional data analysis (e.g., Aitchison, 1986; Aitchison, Barceló-Vidal and Pawlowsky-Glahn, 2002, p. 296) view such analysis as incorrect, however the log-ratio approach itself has not been widely used in archaeometry.

The aim in this paper is to review aspects of the use of log-ratio analysis in archaeometry and to suggest reasons, in addition to ignorance of the methodology, why it may not have been more widely employed. Aitchison, Barceló-Vidal and Pawlowsky-Glahn (2002, p. 302) have pointed out that analysis with log-ratios is essentially equivalent to analysis with logarithms if only trace elements are used. The issues of interest that we wish to discuss thus apply mainly to data sets involving the major and minor oxides, and we focus on glass compositional data for this reason.

Since the examples that we present are ones where log-ratio analysis does not appear to work well in comparison to 'incorrect' methodology, we should emphasize that this paper is not an attempt to argue for the latter and against the former. Rather, we wish to suggest that the structure of certain kinds of archaeometric data is such that common forms of log-ratio analysis will sometimes produce results with no substantive meaning, even when substantively interpretable structure exists. Specifically, the high relative variation of some variables emphasized in a log-ratio analysis may derive, in part, from their low absolute levels, and the variation may be of limited practical interest. This suggests that some form of weighted log-ratio analysis is needed and this is explored in the companion paper (Beardah and Baxter, 2003).

---

[1] In, for example, Aitchison (1986, p. 34) a subcomposition is defined as a subset of variables subjected to a constraining operation so that the row sums are constant. Archaeometric data of the kind under discussion here is not usually so treated, so we shall use the term 'sub-composition' in the way just defined.

2 Log-ratio analysis in archaeometry

The use of ratios or their logarithms in archaeometric data analysis is not new, as Wilson's (1978, p.228) discussion of whether to use concentrations or concentration ratios shows, but is often dictated by archaeometric rather than statistical reasons. One is simply that ratios rather than their concentrations may allow better discrimination between compositional types. Wilson observed that the ratio Sc/Fe had been reported as 'particularly valuable in distinguishing pottery types in several parts of the world'.

The use of ratios can also protect against certain types of analytical error, for example when a sample of artefacts is analyzed in more than one run, and there is systematic instrumental variation between runs (e.g., Pike and Fulford, 1983). In such circumstances two otherwise identical specimens with composition $(x_1\ x_2\ \ldots x_p)$ might be recorded as $(x_1\ x_2\ \ldots\ x_p)$ and $(ax_1\ ax_2\ \ldots\ ax_p)$, for example. Use of the raw measurements would conceal the similarity of the two specimens, whereas in using ratios the instrumental bias, a, 'cancels out'. This is a specific example of what is sometimes called a 'dilution' effect. Other circumstances in which this can occur are when there is differential addition of a neutral temper to a clay in ceramic manufacture (e.g., Leese, Hughes and Stopford, 1989), or natural variation in the clay itself (e.g., Adan-Bayewitz, Asaro and Giauque, 1999).

The paper of Leese, Hughes and Stopford (1989) consciously exploited the log-ratio methodology of Aitchison (1986), which was similarly the inspiration behind Baxter's (1989) advocacy of log-ratio analysis for fully-compositional glass data and Buxeda's (1999) approach to the analysis of ceramic compositions. Subsequent experience led to some waning of Baxter's enthusiasm (Baxter 1993; 1994, p. 74), and the present paper represents a continuing exploration of the reasons for this.

Baxter (1993) was an invited discussion of Tangri and Wright's (1993) dismissal of log-ratio analysis as a usful tool for ceramic compositional analysis. Tangri and Wright's paper is flawed, and the subject of a forceful dismissal by Aitchison, Barceló-Vidal and Pawlowsky-Glahn (2002). The theoretical problems with Tangri and Wright's paper has, however, obscured the fact that they were originally motivated by what appeared to them to be the unsatisfactory practical outcomes of log-ratio analysis, and specifically that less 'correct' approaches led to more useful substantive archaeological interpretation. This is explored, through examples, below and in the companion paper of Beardah and Baxter (2003).

3 Glass compositional data

For illustration, the data of Table 1 are used. The table shows the chemical composition of a subset of 63 colourless Romano-British glass facet-cut beakers, determined by ICPS and expressed as percentages. For convenience, in the table and the paper, oxides are identified by their associated element. The full data set is given in Baxter, Cool and Jackson (2003), where data on three other glass vessel types, cast bowls, wheel-cut beakers and cylindrical cups, are also given. Glass may be formed when sand, soda and lime are fused at a high temperature, and Romano-British glass has a typical soda-lime-silica composition. The dominant component is silica, SiO_2, followed by Na_2O and CaO. These are necessary ingredients in the glass composition and introduced through the choice of raw materials. Silica is introduced through the use of sand, which will also introduce impurities such as Al, Fe, Mg and Ti. Soda may be introduced through the use of soda-rich plant ash or the mineral natron. Lime may be introduced via the sand or as a separate addition.

The colour of a glass reflects both the choice of raw materials and manufacturing technology, including the furnace conditions. As well as entering with the sand Fe, which can affect the colour of the glass in various ways, might also be derived from the crucible used to melt the glass. Owing to impurities the 'natural' colour of glass is often light-blue or light-green (and can be affected

Sample	Al	Fe	Mg	Ca	Na	K	Ti	P	Mn	Sb	Pb	Si
10	1.36	0.58	0.49	4.10	17.68	0.67	0.10	0.05	0.06	2.84	0.39	71.68
11	1.77	0.44	0.54	5.51	18.22	0.51	0.07	0.04	0.02	0.76	0.11	72.01
12	2.20	0.36	0.46	7.29	16.71	0.74	0.05	0.06	0.03	1.59	0.01	70.50
13	1.93	0.34	0.45	6.52	18.17	0.49	0.06	0.04	0.02	1.38	0.02	70.58
14	2.38	0.38	0.42	6.63	17.17	1.01	0.06	0.05	0.03	1.47	0.41	69.99
15	1.96	0.33	0.40	6.68	19.46	0.56	0.05	0.06	0.02	2.84	0.14	67.50
24	1.92	0.27	0.25	4.15	17.84	0.53	0.04	0.04	0.03	1.36	0.29	73.28
25	1.84	0.37	0.37	5.66	19.23	0.65	0.06	0.05	0.02	0.98	0.15	70.62
26	1.90	0.43	0.47	5.62	18.94	0.55	0.08	0.04	0.02	0.99	0	70.96
27	1.82	0.33	0.38	6.31	17.80	0.58	0.06	0.05	0.01	0.65	0.08	71.93
28	1.84	0.36	0.40	4.78	18.15	0.46	0.06	0.04	0.02	1.10	0	72.79
29	1.37	0.57	0.45	3.84	18.20	0.65	0.11	0.06	0.07	2.23	0.32	72.13
40	2.10	0.35	0.32	5.21	16.76	0.57	0.05	0.04	0.01	1.23	0.01	73.35
41	2.03	0.33	0.31	5.00	16.73	0.53	0.05	0.03	0.01	1.19	0.01	73.78
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Table 1: A subset of compositional data for 63 Romano-British colourless facet-cut beakers. Si is obtained by difference.

by the furnace temperature in the manufacturing process). Glass may be deliberately coloured or decoloured through the addition of minerals containing appropriate ingredients, and manganese (Mn) and antimony (Sb) in particular may act as decolourants. There is no general agreement on the levels of these elements needed to represent deliberate addition but, for later reference, we may note that many scholars would regard levels of Mn in the range 0.01–0.05% as representing accidental rather than deliberate addition.

Roman glass is notorious for its compositional homogeneity. The reasons for this are not fully understood and several competing models have been proposed to account for this. In Baxter, Cool and Jackson (2003) the glass was studied with a view to seeing whether or not there were distinct compositional differences between or within vessel types that might throw light on the appropriateness of different models. Figures 1 and 2 are taken from this paper. Types 1 to 4 correspond to cast bowls, facet-cut beakers, wheel-cut beakers and cylindrical cups.

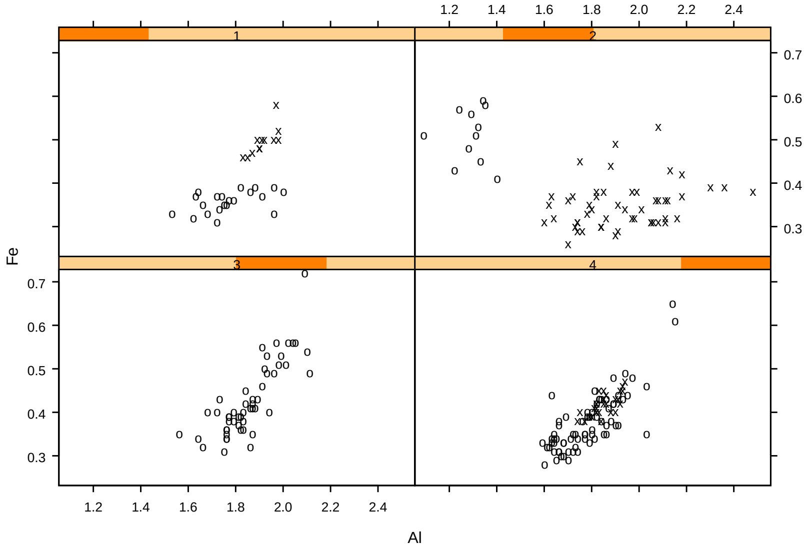

Figure 1: Plots of Fe_2O_3 against Al_2O_3 by type. The use of different labels for types 1, 2 and 4 identifies different compositional groups suggested by bivariate analysis, the subgroups identified for types 1 and 2 being suggested by this plot.

In the top-right panel of Figure 1 it can be seen that there is a distinct compositional group of low Al and relatively high Fe facet-cut beakers, labelled with ‘o’ in the plot, that is also compositionally distinct from other types. Similarly, within the cast bowls at the top-left there appear to be two groups associated with high and low levels of Fe (and Mg and Ca on the evidence of other plots not shown). These phenomena suggest that there are distinct compositional groups within types for which an *archaeological* explanation must be sought. The possibility that different sands were used in the manufacture exists here.

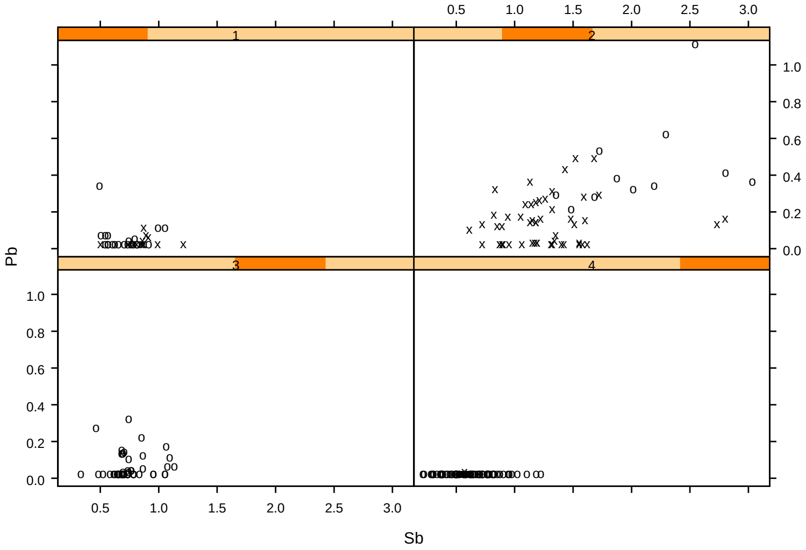

Figure 2: Plots of PbO against Sb_2O_5 by type. The use of different labels for types 1, 2 and 4 identifies different compositional groups suggested by bivariate analysis of other variables.

Figure 2 (top-right) shows that many of the facet-cut beakers have relatively high Pb and/or Sb content that distinguishes them from the other three types. The difference from other types is striking and cannot be accidental, although the reasons for this are not fully understood. It may be noted that the low Al group previously identified includes many of the high Pb and Sb cases. The almost complete absence of Pb at detectable levels for cylindrical cups (bottom-right), type 4, is also worthy of note. This is the latest of the types studied and, together with wheel-cut beakers, included most of the vessels with Mn present at levels of 0.1% or greater.

4 Statistical analysis

Figures 1 and 2 illustrate that there appear to be distinct compositional differences both between and within types, that merit an attempt at explanation. Although these bivariate plots are sufficient to demonstrate this, it could reasonably be required of any multivariate analysis that similar differences be detected. The examples given in this section show that ‘incorrect’ analysis, using PCA of standardized data, does identify these differences, whereas log-ratio analysis does not always do so.

Before presenting these examples some observations on Table 1 are pertinent. Firstly, Si is obtained by difference so that the data are fully compositional. Secondly, 14/63 facet-cut beakers have Pb below the level of detection and recorded as 0. Since Pb helps discriminate between types we ideally wish to retain it in any between-type analysis and, if this is to be based on logarithms, an effective zero-replacement strategy is needed. This is investigated in more detail in Beardah and Baxter (2003). In the present paper all analyses are within-types and, to deal with the problem of zeroes, an ‘other’ variable has been defined as the difference of the first ten variables from 100%

(effectively combining Pb with Si in Table 1). Thirdly, it may be noted that some variables, Ti, P and Mn, are mostly recorded to just one leading digit.

Results of the PCAs to follow will be presented as form biplots (Aitchison and Greenacre, 2002), where the emphasis is on representing the relationship between rows of the data matrix rather than the covariance structure of the variables. This is the usual emphasis in archaeometric practice. Figure 3 shows the results of an 'incorrect' analysis of standardized data, which comfortably suggests the previously noted grouping.

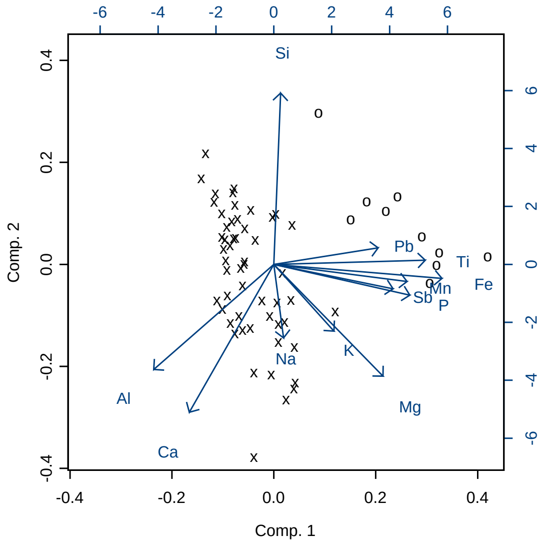

Figure 3: A biplot of the standardized facet-cut beaker data of Table 1, labelled according to the grouping suggested in the top-right of Figure 1.

For the log-ratio analysis we use centered log-ratios of the form

$$y_{ij} = \log[x_{ij}/g(\mathbf{x}_i)]$$

where

$$g(\mathbf{x}_i) = (x_{i1}x_{i2}\ldots x_{ip})^{1/p}$$

is the geometric mean of the data for the ith case. The associated form biplot (when Pb is merged with Si) is shown in Figure 4. The low Al group is suggested in the plot, though not as clearly as in the previous figure. It can be seen that the plot is dominated by (ratios relative to) Mn and Sb, and the group is successfully separated out largely because the low Al cases are also high Sb. In fact the plot is not too dissimilar from a simple plot of Sb against Mn.

It can be argued that this analysis is not too bad, but we can do worse. Figure 5 shows a similar analysis for the cast bowl data, type 1. This fails to suggest the grouping evident in the top-left of Figure 1, although such a grouping is evident in a biplot of standardized data. The plot is once again dominated by Mn and Sb and very similar to a simple bivariate plot of these two variables. The striated pattern arises because Mn only takes the values 0.01, 0.02, 0.03 and 0.04%

5 Discussion

The examples of the previous section are intended to show that log-ratio analysis may fail to recover structure in the data or fail to do so clearly, even when interpretable archaeological structure exists.

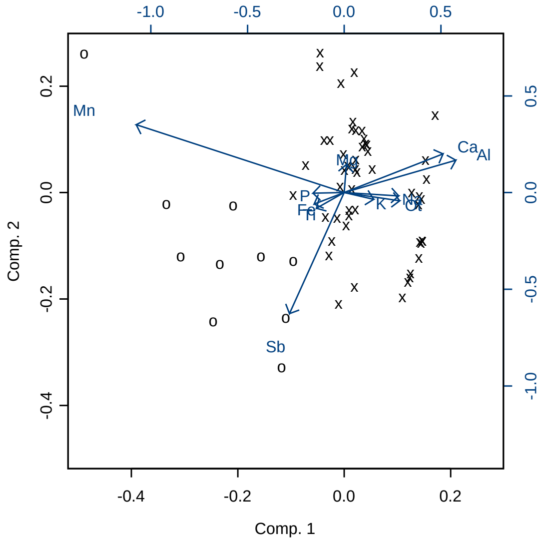

Figure 4: A biplot of the log-ratioed data of Table 1, labelled according to the grouping suggested in Figure 1.

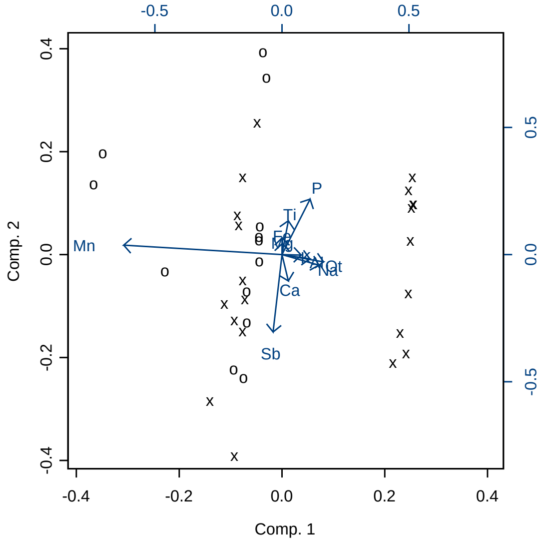

Figure 5: A biplot of the log-ratioed data of vessel type 1, labelled according to the grouping suggested in Figure 1.

At the same time, 'incorrect' analysis such as the PCA of standardized data does recover structure. These results are not pathological. Log-ratio analysis of types 3 and 4 is also dominated by Mn and Sb, and largely equivalent to a bivariate plot of them. Experimentation with log-ratio analysis can recover the structure evident from simpler plots, but only after additionally merging variables such as Mn, Sb and P into the 'other' category (see Baxter, Cool and Jackson, 2003, for an example).

What is happening and what can be done about it? Log-ratio analysis is promoted (among other reasons) for emphasizing relative variation at the expense of absolute variation, and 'incorrect' approaches are decried (among other reasons) for doing the opposite. The problem with data of the kind we have been using is that substantive meaning may sometimes be attributed to absolute variation, but is ignored in a log-ratio analysis. Conversely, variables with high relative variation may be emphasized but there may be no associated substantive interpretation.

This is most evident with respect to manganese, which dominates log-ratio analyses of all four vessel types. Its lowest value is 0.01% for each data set but, except for vessel type 4 and some outliers, values in excess of 0.04% are uncommon. These low absolute values and variation are entirely consistent with natural levels of impurity in the raw materials of production, but the high relative variation compared to other variables means that it is over-emphasized in the log-ratio analyses, producing results that have no useful substantive interpretation.

This is just a manifestation of the well-known problem with PCA, that analyses will be dominated by a subset of high variance variables, if such exist. In 'standard' PCA the usual way of dealing with this is to standardize variables to have equal variance. This seems not to be done in comparable applications of log-ratio analysis of which we are aware (and to do so would negate the emphasis on relative variation that log-ratio analysis exploits). An alternative is to try and retain the principles of correct compositional data analysis, but downweight the influence of variables having high relative variation largely as a consequence of their low absolute presence. That is, some form of weighted log-ratio analysis is needed. This is the thinking behind the ratio-map approach to analysis developed by Greenacre (2002), and it is explored empirically in Beardah and Baxter (2003).

Acknowledgments

We are grateful to The British Academy and NERC for funding the analytical programme that generated the data used in the paper.

References

Adan-Bayewitz, D., Asaro, F., and Giauque, R.D., 1999, Determining pottery provenance – application of a new high-precision X-ray fluorescence method and comparison with instrumental neutron activation analysis: Archaeometry v. 41, p. 1-24.

Aitchison, J., 1986, The statistical analysis of compositional data: Chapman and Hall, London, 416 p.

Aitchison, J., and Greenacre, M., 2002, Biplots of compositional data: Applied Statistics v. 51, p. 375-392.

Aitchison, J., Barceló-Vidal, C., and Pawlowsky-Glahn, V., 2002, Some comments on compositional data analysis in archaeometry, in particular the fallacies in Tangri and Wright's dismissal of logratio analysis: Archaeometry v. 44, p. 295-304.

Baxter, M.J., 1989, Multivariate analysis of data on glass compositions: a methodological note: Archaeometry v. 31, p. 45-53.

Baxter, M.J., 1993, Comment on D.Tangri and R.V.S. Wright, ‘Multivariate analysis of compositional data . . .’: Archaeometry v. 35, p. 112-115.

Baxter, M.J., 1994, Exploratory multivariate analysis in archaeology: Edinburgh University Press, Edinburgh, 307 p.

Baxter, M.J., Cool, H.E.M., and Jackson, C.J. 2003, Further studies in the compositional variability of colourless Romano-British glass: (in preparation).

Beardah, C.C., and Baxter, M.J., 2003, Compositional data analysis of archaeological glass – problems and possible solutions: (in preparation).

Bieber, A.M., Brooks, D.W., Harbottle, G., and Sayre, E.V., 1976, Application of multivariate techniques to analytical data on Aegean ceramics: Archaeometry v. 18, p. 59-74.

Buxeda i Garrigós, J., 1999, Alteration and contamination of archaeological ceramics – the perturbation problem: Journal of Archaeological Science v. 26, p. 295-313.

Greenacre, M.J., 2002, Ratio maps and correspondence analysis: Departament d’Economia i Empresa, Universitat Pompeu Fabra, Working Paper 598. (http://www.econ.upf.es/cgi-bin/onepaper?598)

Leese, M.N., Hughes, M.J., and Stopford, J., 1989, The chemical composition of tiles from Bordesley, in Rahtz, S., and Richards, J., eds., Computer applications and quantitative methods in archaeology 1989: British Archaeological Reports, Oxford, p. 241-249.

Pike, H.H.M., and Fulford, M.G., 1983, neutron activation analysis of black-glazed pottery from Carthage: Archaeometry v. 25, p. 77-86.

Tangri, D., and Wright, R.V.S., 1993, Multivariate analysis of compositional data: applied comparisons favour standard principal components analysis over Aitchison’s loglinear contrast method: Archaeometry v. 35, p. 103-112.

Wilson, A.L., 1978, Elemental analysis of pottery in the study of its provenance – a review: Journal of Archaeological Science v. 5, p. 219-236.