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Research Paper

Stochastic modelling of multi-grain equivalent dose (D_e) distributions: Implications for OSL dating of sediment mixtures

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A B S T R A C T

A number of recent optically stimulated luminescence (OSL) studies have cited post-depositional mixing as a dominant source of equivalent dose (D_e) scatter across a range of sedimentary environments, including those previously considered 'best suited' for OSL dating. The potentially insidious nature of sediment mixing means that this problem may often only be identifiable by careful statistical analysis of D_e data sets. This study aims to address some of the important issues associated with the characterisation and statistical treatment of mixed D_e distributions at the multi-grain scale of analysis, using simulated D_e data sets produced with a simple stochastic model. Using this Monte Carlo approach we were able to generate theoretical distributions of single-grain D_e values, which were then randomly mixed together to simulate multi-grain aliquot D_e distributions containing a known number of mixing components and known corresponding burial doses. A range of sensitivity tests were undertaken using sediment mixtures with different aged dose components, different numbers of mixing components, and different types of dose component distributions (fully bleached, heterogeneously bleached and significantly overdispersed D_e distributions). The results of our modelling simulations reveal the inherent problems encountered when dating mixed sedimentary samples with multi-grain D_e estimation techniques. 'Phantom' dose components (i.e. discrete dose populations that do not correspond to the original single-grain mixing components) are an inevitable consequence of the 'averaging' effects of multi-grain D_e analysis, and prevent the correct number of mixing components being identified with the finite mixture model (FMM) for all of the multi-grain mixtures tested. Our findings caution against use of the FMM for multi-grain aliquot D_e data sets, even when the aliquots consist of only a few grains.

1. Introduction

A number of sources of variation can contribute to the commonly observed scatter in equivalent dose (D_e) distributions of sedimentary samples, including heterogeneous bleaching of grains prior to burial (e.g. Olley et al., 2004a), post-depositional mixing of grains from adjacent sedimentary layers (e.g. Roberts et al., 1998a), beta-dose heterogeneity in the natural burial environment (e.g. Olley et al., 1997), measurement and instrument uncertainties (e.g. Thomsen et al., 2005), and intrinsic grain-to-grain variability in luminescence behaviour and differing responses to fixed SAR conditions (e.g. Jacobs et al., 2003b). Sediment mixing by post-depositional processes has been cited as a dominant source of D_e variability across a range of archaeological and sedimentary environments (e.g. Roberts et al., 1998b, 1999; Heimsath et al., 2002; Spencer et al., 2003). Furthermore, a number of recent single-grain optically stimulated luminescence (OSL) studies have revealed that sediment mixing can be a significant problem in depositional contexts previously thought to be 'best suited' for OSL dating, such as quartz-dominated, well-bleached, aeolian, dryland sediments (e.g. Duller et al., 2000; Feathers, 2003; Bateman et al., 2003; Carr et al., 2007). Bateman et al. (2007a) found that field identification of sediment mixing is often difficult because the absence of depositional bedding structure is not necessarily indicative of sediment mixing, whilst the presence of sedimentary structure does not necessarily preclude post-depositional disturbance. This study aims to address some of the important issues associated with the analysis of mixed D_e distributions, using simulated D_e data sets produced with a simple stochastic model.

Sediment mixing can arise from a number of post-depositional processes and can result in the multi-directional translocation of grains between adjacent depositional layers. Sediment mixing, therefore, has the potential to affect the appearance of D_e distributions in a wide variety of ways: by symmetrically increasing the overall spread of D_e values, or by increasing either positive skewness (where the dominant intrusion is by younger grains) or negative skewness (where the intrusive grains are mostly older), or by

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creating discrete dose populations (including zero-age grains) and multi-modal D_e distributions. The signature of post-depositional mixing can, in principle, be determined at the single-grain scale of analysis, as individual grains that have intruded from younger or older units may be identified as discrete components in a D_e distribution. At the multi-grain scale of analysis, however, the signatures of minor sedimentary mixing are apt to be confused, as individual D_e estimates are obtained from aliquots containing several tens, hundreds, or even thousands of grains. The presence of younger or older intrusive grains may therefore become 'masked' in the final D_e estimates of individual aliquots that contain an assortment of both younger/older intrusive grains and *in situ* grains. These 'averaging' effects of multi-grain analysis have important implications for our ability to obtain reliable burial age estimates from mixed sediments using aliquots composed of more than one grain. The modelling simulations undertaken in this paper aim to address this issue directly.

A number of statistical treatments have been proposed to obtain representative burial dose estimates from post-depositionally mixed sediments (e.g. Roberts et al., 2000; Spencer et al., 2003; Sivia et al., 2004). The finite mixture model (FMM) of Galbraith and Green (1990) and Galbraith and Laslett (1993) (reviewed by Galbraith, 2005) is one of the most mathematically rigorous of these approaches, and it has been used in a number of recent OSL studies of mixed sediments (e.g. Roberts et al., 2000, 2001; Jacobs et al., 2006a, 2008b; David et al., 2007; Bateman et al., 2007b). This age model is designed to identify discrete populations within single-grain D_e data sets containing multiple dose components, and provides estimates of the number of dose components, their corresponding doses, and the relative proportion of each component present. The accuracy and applicability of the FMM has been validated using a series of 'synthetic' mixtures of grains (i.e. composites created prior to, or after, D_e determination), whose component doses and mixing proportions are well-constrained (e.g. Roberts et al., 2000). It is also possible to use modelling simulations (e.g. Bailey and Arnold, 2006) to generate theoretical distributions of D_e values that can be mixed together to create 'simulated synthetic' mixtures. With this method, large numbers of D_e values can be generated rapidly, and a range of different mixing parameters can be controlled and varied systematically, to test for age model suitability across a wide range of D_e distribution types. The latter approach is adopted in the present work.

The FMM originally described by Galbraith and Green (1990), and extended to OSL dating by Roberts et al. (2000), was designed for application to mixed populations of *individual* mineral grains. However, some studies have applied the FMM to multi-grain OSL data sets (e.g. Rodnight et al., 2006). In this paper, the term 'multi-grain' refers to an individual aliquot consisting of several grains that are measured simultaneously, or a specially made disc drilled with an array of holes, in each of which more than one grain is contained (e.g. Feathers et al., 2006a; Porat et al., 2006). The present study makes use of modelled synthetic mixtures to assess (i) the structure of mixed multi-grain D_e data sets compared to the true single-grain D_e distributions, and (ii) the degree of bias associated with FMM applications to multi-grain D_e data sets.

2. The model

This research follows the approach of Bailey and Arnold (2006), but uses a simpler stochastic model to generate multi-grain aliquot D_e values from Monte Carlo sampling of simulated single-grain D_e data sets. The input for the model is a series of theoretical end-member single-grain D_e values, which, although simplistic, is sufficient for the purpose of the present study – the focus of which is not the origins of the single-grain D_e values but the resultant multi-grain D_e distributions generated from these single-grain estimates.

The stochastic model works as follows: randomly generated single-grain D_e values are first sampled from parent distributions of theoretical D_e values, and then combined together in randomly determined quantities to create simulated multi-grain D_e values. Each iteration of the multi-grain D_e simulation is repeated 100 times for each modelling scenario in order to build up a randomly sampled population of 100 individual multi-grain D_e values. This provides a statistically significant number of multi-grain D_e values with which to assess the suitability of the FMM, and represents a similar sample size to that ideally measured for empirical multi-grain OSL samples. We expand on the main elements of this simple model below. Table S1 summarises the main parameters of the model, as well as other parameters and variables mentioned in the text.

2.1. Monte Carlo sampling of single-grain D_e values from parent distributions

To simulate mixed-dose distributions, the modelling process starts with the generation of individual single-grain D_e values that have been selected randomly from two or more log-normal parent distributions (P_i), whose probability at a given D_e value is given by the equation:

$$p(D_e) = \frac{1}{D_e \sigma_{Pi} \sqrt{2\pi}} \exp\left(\frac{-[\ln(D_e) - \mu_{Pi}]^2}{2\sigma_{Pi}{}^2}\right) \quad (1)$$

where μ_{Pi} represents the mean D_e (Gy) of the *i*th single-grain parent D_e distribution, and σ_{Pi} is the standard deviation of the *i*th single-grain parent D_e distribution. Log-normal parent D_e distributions were chosen instead of normal (Gaussian) D_e distributions, as a certain degree of positive skewness should be the general expectation for the majority of empirical single-grain D_e distributions, including those of samples that had been fully bleached prior to burial and not affected by post-depositional mixing (Galbraith, 2003). This is a direct consequence of the inherent error properties of single-grain D_e distributions, which tend to be multiplicative rather than additive (Roberts and Galbraith, in press) – that is, the absolute standard error of the individual D_e estimates tends to increase with the size of the D_e estimate (e.g. Fig. 1c). This type of error relationship reflects the increasing significance, in absolute terms, of certain experimental uncertainties as D_e increases (in particular, instrument reproducibility errors and dose–response curve-fitting errors). Such error distributions tend to produce positively skewed distributions of empirical D_e values, since larger D_e values will naturally scatter more than smaller ones. Positively skewed or log-normal D_e distributions, therefore, should be expected for samples with D_e values derived from the linear part of the dose–response curve (e.g. Roberts and Galbraith, in press), and the extent of positive skewness is likely to be accentuated in samples with sensitivity-corrected natural OSL signals that fall on the non-linear part of the regenerated OSL dose–response curve. The FMM assumes that the log D_e estimates of each dose component in a given sediment mixture are normally distributed, so the use of log-normal parent D_e distributions is arguably more appropriate for simulating younger as well as older sediment mixtures (e.g. those simulated in Experiments 1c, 1d and 2c) and mixtures affected by additional sources of scatter, such as partial bleaching and beta-dose heterogeneity (e.g. those simulated in Experiments 3c and 3d).

2.2. Assigning error terms to the sampled single-grain D_e values

Relative errors were selected randomly from a log-normal parent distribution that has been fitted to an empirical data set of