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A new R function for the Internal External Uncertainty (IEU) model

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Abstract

A new function (*calc_IEU*) is now available in the latest version of the R Luminescence package (version 0.4.2). The *calc_IEU* function can be used to calculate an equivalent dose (D_e) value for a given dose distribution using the Internal External Uncertainty (IEU) model. The IEU model is used in luminescence dating to determine a D_e value for a partially-bleached sample by calculating the weighted mean from the well bleached part of a partially-bleached population. The new *calc_IEU* function automates the calculation of the IEU model so that the results are produced rapidly and reproducibly. This is advantageous as the user can easily perform sensitivity tests of the model in response to changing input parameters.

Keywords: R, luminescence dating, Internal External Uncertainty (IEU) model, single grains

1. Introduction

The Internal External Uncertainty (IEU) model can be used to determine an equivalent dose (D_e) value for luminescence dating of a partially-bleached sample (Thomsen et al., 2007). The D_e value is calculated as the weighted mean from the grains in a partially-bleached population that the IEU model identifies to have been well bleached upon deposition. The IEU model has been successfully used in a number of studies to provide D_e values for sedimentary samples using both single grains and multiple grains (e.g. Reimann et al., 2012; Medialdea et al., 2014; Sim et al., 2014). A new function that automates the calculation of the IEU D_e value is now available in the latest version of the R Luminescence package (version 0.4.2; Kreutzer et al., 2012). The *calc_IEU* function aims to automate the calculations of the IEU model for luminescence dating, in addition to providing output features that rapidly assess the sensitivity of the IEU model to changing input parameters. The purpose of this work is to explain the calculations of the *calc_IEU* function and provide a worked example of the function using D_e values determined for single grains of quartz from a glaciofluvial sample taken from the U.K. that was partially bleached upon deposition (sample T4CEIF01; Fig. 1a).

2. The IEU model

The IEU model is based on the assumption that the well-bleached grain population in the dose distribution from a poorly-bleached sample is normally distributed, and that this population can be identified if the uncertainties assigned to individual dose estimates adequately describe the observed variability. It is standard practise to determine the uncertainties on individual D_e values from intrinsic sources (i.e. counting statistics, the instrument reproducibility and the dose-response curve fitting). Extrinsic factors such as heterogeneity of the beta dose-rate for individual grains may also cause variability in a dataset. Ideally, the uncertainty arising extrinsically for a given suite of samples is determined from a sample that has been well bleached in the natural environment, meaning that factors such as microdosimetry are considered within the uncertainty estimate. However, it is often difficult to determine this information for all samples due to the lack of analogue well-bleached sediments in certain depositional settings (e.g. glaciofluvial). Alternatively, Thomsen et al. (2007) use a number of gamma dose-recovery experiments, administering progressively larger given doses to measure the minimal amount of scatter expected in a well-bleached D_e distribution. The authors plot the absolute overdispersion values (in Gy) determined from these experiments against the CAM D_e values and fit a linear function to the data to determine the change in overdispersion with in-

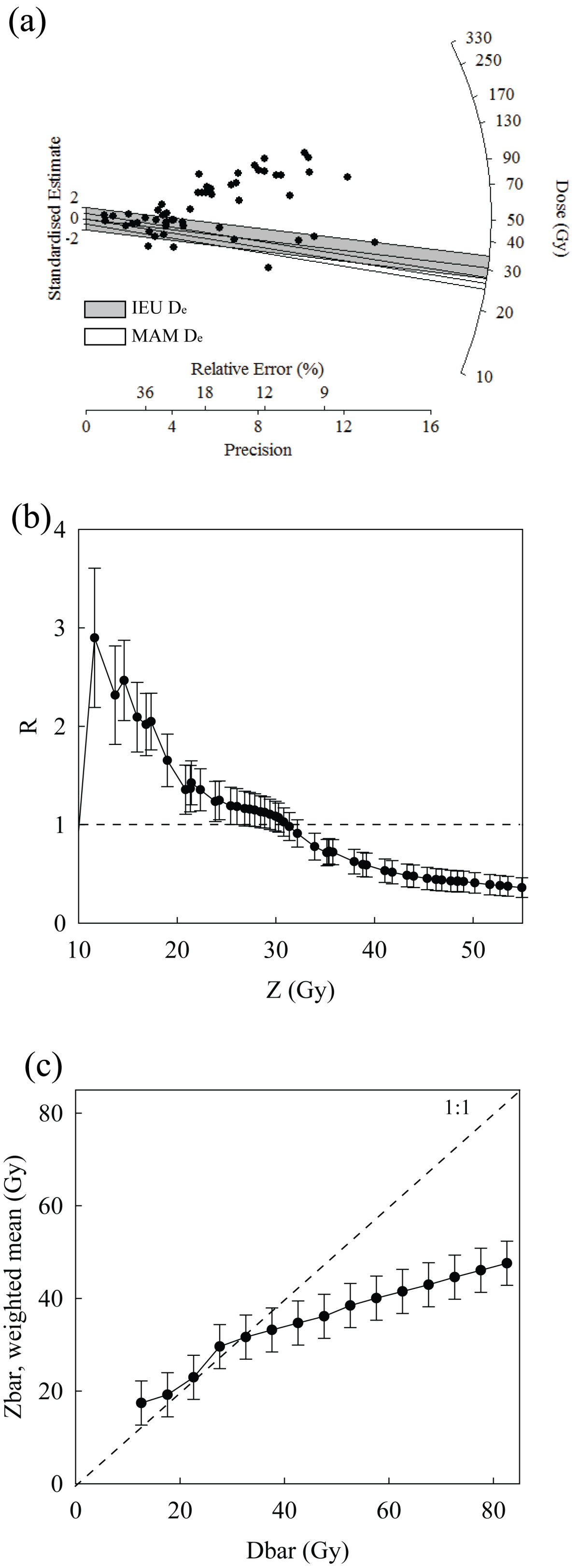

Figure 1. Results from applying the IEU model to D_e values determined from single grains of quartz from a partially-bleached sample taken from a glaciofluvial setting in the U.K. (sample T4CEIF01): (a) the D_e values are presented in a radial plot; (b) the values of R calculated for the final iteration of *Dbar* when determining the IEU D_e value for this dataset are plotted against Z; and (c) the output plot from calculating *Zbar* using fixed values of *Dbar* when a = 0.3

creasing given dose. In the IEU model the slope of this linear function is termed the *a* value, which by definition is similar to the σ_b value in the Minimum Age Model (MAM; Galbraith et al., 1999), while the intercept provides the *b* value, which defines how much overdispersion is expected in a D_e distribution for a 0 Gy dose (e.g. the absolute overdispersion which can be obtained from thermal transfer experiments).

The uncertainty on each individual D_e value can then be calculated using the uncertainty arising from counting statistics (σ_c^2), the *a* and *b* values, and the burial dose (*Dbar*) in Eq. 1 (Thomsen et al., 2007).

$$\sigma_{tot} = \sqrt{\sigma_c^2 + (a \cdot Dbar + b)^2} \tag{1}$$

The value of *Dbar* in Eq. 1 is initially unknown and so Thomsen et al. (2007) suggest that it should be solved using an iterative approach. To iterate *Dbar*, an initial *Dbar* value is substituted into Eq. 1, and the total uncertainty assigned to each D_e value is calculated (σ_{tot}). The internal/external consistency criterion (Eqs. 2, 3 and 4) is then used to determine which grains (or aliquots) from the partially-bleached population were well bleached upon deposition (Thomsen et al., 2003). The weighted mean dose (termed *Z*) of the identified well-bleached part of the partially-bleached population is then calculated and compared to the value of *Dbar*. If *Z* is not equal to *Dbar*, the calculation of *Z* is repeated again using a new value of *Dbar*. This iteration process is continued until *Z* is equal to *Dbar*, where *Z* is calculated using only the grains (or aliquots) that are deemed to form the well-bleached part of the partially-bleached distribution (i.e. R = 1, see below). This value of *Z* that is equal to *Dbar* is the burial dose determined for this sample (termed the IEU D_e value in the *calc_IEU* function).

To calculate the internal/external consistency criterion the D_e values in a given distribution are first ranked from the smallest D_e value to the largest D_e value. Eq. 2 is then used to calculate the weighted mean (*Z*), where D_i are the individual D_e values, σ_{i} are the individual estimates of uncertainty for D_i and N is the total number of D_i.

$$\mathrm{Z} = \frac{\sum_{\mathrm{i}=1}^{\mathrm{N}} \mathrm{D_i} / \sigma_{\mathrm{i}}^2}{\sum_{\mathrm{i}=1}^{\mathrm{N}} 1 / \sigma_{\mathrm{i}}^2} \tag{2}$$

The standard error of *Z* is then calculated in two ways: (1) as an internal measure ($\alpha^2{}_{in}$) which is dependent upon how much variation there is within the counting statistics (Eq. 3); and (2) as an external measure ($\alpha^2{}_{ex}$) which also is dependent upon how much variation arises from each individual D_e estimate varying from the mean (Eq. 4) (Topping, 1955; Thomsen et al., 2003).

$$\alpha_{\mathrm{in}}^2 = \frac{1}{\sum_{i=1}^{N} 1 / \sigma_i^2} \tag{3}$$

$$\alpha_{\mathrm{ex}}^2 = \frac{\sum_{i=1}^{N} (D_i - Z)^2 / \sigma_i^2}{(N-1) \sum_{i=1}^{N} 1 / \sigma_i^2} \tag{4}$$

Using these measures, the internal/external consistency criterion can be calculated from $R = \alpha^2{}_{in} / \alpha^2{}_{ex}$, where the uncertainty on R is $(2(n-1))^{-0.5}$ and n is the number of data points used for the calculations. R is calculated cumulatively, starting with the lowest two D_e values and finishing with including all the D_e values into the calculation. All the grains (or aliquots) included in the calculation of an R value ≥ 1 are deemed to form the well bleached part of the partially-bleached population (e.g. Fig. 1b), and Z is calculated from only these grains (or aliquots).

3. The *calc_IEU* function: a worked example

The *calc_IEU* function works in a similar way to the existing age models built into the R 'Luminescence' package. It first requires the input of a data frame containing two columns; (1) the D_e values and (2) the uncertainties of the D_e values. Input variables (or arguments) are also required to define the parameters used for the calculations in the function (e.g. *a* and *b*). The following section works through an example of how to use the *calc_IEU* function and what outputs are produced. Fig. 1a shows a radial plot containing the D_e values for the example dataset determined from single grains of quartz from a glaciofluvial sample, which was partially bleached upon deposition. The individual estimates of uncertainty assigned to each D_e value shown in Fig. 1a are based on counting statistics, instrument reproducibility (measured as 2.5 %) and dose-response curve fitting. Similar to the σ_b value in MAM, accurate estimates of *a* and *b* values need to be considered for each sample. The uncertainty arising extrinsically for this sample was estimated from the overdispersion value determined for a sample from this environment that was naturally well bleached upon deposition; *a* and *b* values for this sample were estimated to be 0.30 and 0.01, respectively. To call the *calc_IEU* function the user is required to adapt the arguments written below, defining the correct input parameters where necessary (e.g. *a* and *b* values).

```
calc_IEU(data = data, a = 0.30, b = 0.01, interval
    = 5, trace = FALSE, verbose = TRUE, plot =
    TRUE)
```

data	**data.frame** (required): containing two columns; D_e and D_e uncertainties
a	**numeric** (required): slope (e.g. 0.30)
b	**numeric** (required): intercept (e.g. 0.01)
interval	**numeric** (required): interval used for fixed iteration of Dbar (e.g. 5 Gy)
trace	**logical**: print iteration of Dbar to screen (TRUE/FALSE)
verbose	**logical**: console output (TRUE/FALSE)
plot	**logical**: plot output (TRUE/FALSE)

Before the IEU D_e value is determined for a D_e distribution, the *calc_IEU* function will automatically calculate Z using fixed values of *Dbar* to assess whether there is more than one solution where Z = *Dbar* (R = 1). Output plots of the results are provided to allow for comparisons if the user wishes to compare the influence of changing input parameter (e.g. *a*) or the characteristics of D_e distributions determined for different samples. Note that when performing the calculations of Z using a fixed value of *Dbar*, Z is referred to as *Zbar* to differentiate these calculations from the automatic iteration of *Dbar* used to calculate the IEU D_e value. The fixed values of *Dbar* range from an upper limit defined as the mean of the D_e distribution to a lower limit set as the lowest D_e value in the dataset. The *calc_IEU* function automatically determines the fixed values of *Dbar* from the upper limit to the lower limit by repeatedly subtracting the value defined in Gy by the argument *interval*. The size of the interval used will depend on the range of the D_e distribution. If the range in the D_e distribution is small then it would be advantageous to use smaller intervals to improve the resolution of the calculations. The calculations from using fixed values of *Dbar* to calculate *Zbar* are provided in an output table (e.g. Table 1), and the fixed values of *Dbar* are plotted against *Zbar* in an output plot (e.g. Fig. 1c).

Table 1 shows an example of what happens for the calculations when using fixed values of *Dbar*. The mean is first calculated for the D_e distribution, here it is 82.59 Gy, the fixed interval in Gy (i.e. 5 Gy) is then subtracted to determine the first *Dbar.fixed* value of 77.59 Gy. This *Dbar.fixed* value is then used to calculate R and determine how many grains form the well-bleached part of the D_e distribution. The weighted mean (*Zbar*) of these grains is then calculated and plotted against *Dbar.fixed* (e.g. Fig. 1c). The *calc_IEU* function will then automatically subtract 5 Gy from the present value of *Dbar* (i.e. 77.59 Gy) to set a new value of *Dbar.fixed* (i.e. 72.59 Gy) used to calculate the next value of *Zbar*. This process continues to be repeated until the function identifies that the value of *Dbar.fixed* is set as a value lower than the lowest D_e value, whence the *calc_IEU* function will cease calculations.

The fixed iteration of *Dbar* in Fig. 1c demonstrates that there are multiple solutions ranging from 17.6 to 32.6 Gy where *Dbar* = Z and R = 1 for the example dataset used in this study, even though the final solution is determined to be (31.13 ± 2.54) Gy (see Table 2). In such cases, the IEU D_e value is the lowest value of Z that is equal to *Dbar*, because the model aims to determine a minimum dose from this D_e distribution. Given that there may be multiple solutions of the IEU model for some data sets, it is important that the automatic iteration of *Dbar* used to calculate the IEU D_e value begins by setting the first *Dbar* value equal to the lowest D_e value in the dataset and iterating to larger values of *Dbar*. Subsequent iterations of *Dbar* then automatically set Z that was calculated during the previous iteration as the new *Dbar*, and repeat the iterations until *Dbar* = Z where R = 1.

The argument *trace* allows the user to print the results to the screen from the iterations of *Dbar* to calculate the IEU D_e value. The calculations of Z, α^2_{ex}, α^2_{in} and R used for the final iteration of *Dbar* that determines the IEU D_e value are provided in an output file, and the weighted mean (Z) is plotted against R in an output plot (e.g. Fig. 1b). A summary of the results from the IEU model are provided in an output

Dbar	Dbar.Fixed	Zbar	Zbar.Error	n	R	a	b
82.59	77.59	47.60	4.76	37	0.97	0.30	0.01
77.59	72.59	46.07	4.76	36	0.98	0.30	0.01
72.59	67.59	44.60	4.76	36	0.93	0.30	0.01
67.59	62.59	42.95	4.76	34	0.99	0.30	0.01
62.59	57.59	41.50	4.76	34	0.94	0.30	0.01
57.59	52.59	40.06	4.76	33	0.95	0.30	0.01
52.59	47.59	38.47	4.76	32	1.00	0.30	0.01
47.59	42.59	36.14	4.76	29	0.94	0.30	0.01
42.59	37.59	34.68	4.76	28	0.95	0.30	0.01
37.59	32.59	33.20	4.76	28	0.87	0.30	0.01
32.59	27.59	31.64	4.76	27	0.93	0.30	0.01
27.59	22.59	29.61	4.76	23	1.00	0.30	0.01
22.59	17.59	22.96	4.76	13	0.96	0.30	0.01
17.59	12.59	19.21	4.76	9	0.86	0.30	0.01
12.59	7.59	17.43	4.76	8	0.90	0.30	0.01

Table 1. Fixed iteration of *Dbar* determined for the example dataset using an *a* value of 0.30. The number of grains/aliquots determined to form the well-bleached part of the partially-bleached population is shown as *n*

file (e.g. Table 2), and contains the values for *Dbar, Z* (now referred to as the IEU D_e), the uncertainty on the D_e value, the number of D_e values defined as the well-bleached part of the partially-bleached population, and the *a* and *b* values used for the calculations. For the example dataset given in Fig. 1a, the IEU D_e value (31.13 Gy $\pm$ 2.54 Gy) determined using an *a* value of 0.30 was consistent with the MAM D_e value of (26.51 Gy $\pm$ 4.99 Gy), which was calculated using a σ_b value of 0.30 (Fig. 1a). An example of an R script that a user can copy to call the *calc_IEU* function and save the output files is shown below (after Burow, Pers. Comm.).

```
## Load library
library("Luminescence")
## Input data
setwd("C:/Users/Documents/R/EXAMPLE")
data <- read.table("Example.txt", header = F)
## Calculate the IEU model
pdf(paste0("IEU_Plots.pdf"))
IEU <- calc_IEU(data = data, a = 0.30, b = 0.01,
    interval = 5, trace = FALSE, verbose = TRUE,
    plot = TRUE)
dev.off()
## Write tables
tables <- get_RLum.Results(IEU, "tables")
for(i in seq_along(tables)) {
write.table(tables[[i]], file = paste0(names(
    tables)[i], ".txt"))
}
```

Dbar	IEU.D_e (Gy)	IEU.Error (Gy)	Number of D_e	a	b
31.13	31.13	2.54	26	0.3	0.01

Table 2. Results from calculating the IEU model for the example dataset shown in Fig. 1a.

Although it is not the case for the example dataset shown in this study, the IEU model may not always be able to determine a D_e value using the input parameters provided, and an error message will be produced by the *calc_IEU* function. It is likely that an error message is provided because the population of grains that are deemed to form the well bleached part of the partially-bleached distribution is less scattered than can be explained by the value of *a*. In such cases, it is likely that the value of *a* is too large and overestimates the amount of scatter in a D_e distribution determined from a well-bleached sample of this material; thus, the value of *a* needs revising for the IEU model to be able to calculate a D_e value for this sample.

4. Sensitivity of the IEU model to changing parameters

The outcome of any minimum age model that accounts for the uncertainties on individual D_e values (e.g. the IEU model and MAM) is critically dependent upon the accuracy of the individual uncertainties assigned. Where the assigned uncertainties are overestimated, such a statistical model will overestimate the number of grains that form the well-bleached part of the D_e distribution, and consequently overestimate the D_e value. Similarly, if the assigned uncertainties are too small then too few of the grains are determined to have been well-bleached upon deposition and the D_e value is underestimated. The uncertainties assigned to the individual D_e estimates must therefore be as accurate as possible in order to provide accurate D_e values for a given D_e distribution; this includes using appropriate estimates of *a* and *b* for the IEU model.

A major advantage of the *calc_IEU* function is that a rapid assessment of the sensitivity of the IEU model to different parameters (e.g. *a*) can be provided. This can be a useful tool for luminescence dating of sedimentary samples from the natural environment because it is often difficult to determine the amount of scatter arising from extrinsic factors, such as external microdosimetry. Previous studies using single-grain and multiple-grain dating of quartz have reported that the

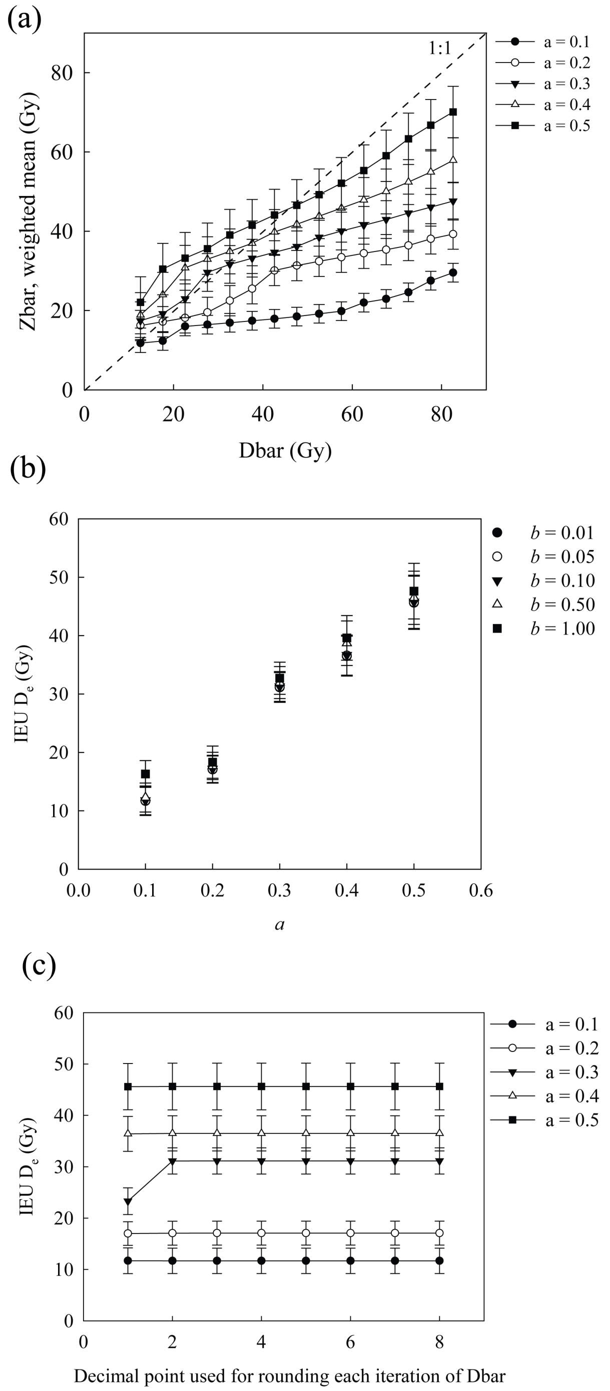

Figure 2. Results from applying the IEU model and changing different parameters for the example datasets: (a) fixed iteration of *Dbar* using a range of *a* values; (b) IEU D_e values calculated when varying both the *a* and *b* values; (c) IEU D_e values determined when the values of *Dbar* and *Z* are calculated to different decimal points for comparison using different *a* values.

sensitivity of the IEU D_e value to changing values of *a* can be different for D_e distributions determined from different samples (Medialdea et al., 2014; Sim et al., 2014). The example dataset (Fig. 1a) is used in this study to test how sensitive the IEU model is to varying the values of *a* and *b*, and the number of decimal points that the values of *Dbar* and *Z* are calculated to for comparison. The results from performing fixed iterations of *Dbar* when changing the *a* value from 0.1 to 0.5 are shown in Fig. 2a, and suggest that the fixed iteration of *Dbar* using an *a* value of 0.3 is the only dataset that has multiple solutions for *Dbar* = *Zbar*. Fig. 2a plots the corresponding IEU D_e values calculated when automating the iteration of *Dbar* using *a* values from 0.1 to 0.5, in addition to simultaneously varying the value of *b* from 0.01 to 1.00. These sensitivity experiments demonstrate that the IEU D_e value for this sample is highly sensitive to changes in the value of *a* value but less sensitive to changes in the value of *b*. This is because the value of *b* only becomes important for the calculations when the D_e distributions contain several low D_e values, which is not the case for the sample shown in Fig. 2. The differences in the IEU D_e values in Fig. 2 emphasise the need to accurately quantify the amount of scatter in a naturally well-bleached D_e distribution for this material, which is also an important requirement when applying the MAM.

The number of decimal points that the values of *Dbar* and *Z* are calculated to for comparison is also varied for the example dataset to assess whether this influenced the calculation of the IEU D_e value (Fig. 2c). The results from varying the number of decimal points from one to eight show how it did not affect the IEU D_e value for the majority of cases. However, the IEU D_e value calculated using an *a* value of 0.3 was lower when *Dbar* and *Z* were calculated to one decimal point (23.3 Gy ± 2.6 Gy), in comparison to when it was calculated to two decimal points (31.13 Gy ± 2.54 Gy). Although this is a very minor part of the calculations of the IEU model, Fig. 2c shows that it can have a large impact upon the D_e value determined. As a result, the *calc_IEU* function is designed to consistently calculate *Dbar* and *Z* to two decimal points for comparison to ensure that all results are reproducible.

5. Conclusions

A new function (*calc_IEU*) is now available in the R 'Luminescence' package and can be used to calculate burial dose estimates for a given D_e distribution. The IEU model can be used to determine D_e values for luminescence dating of partially-bleached samples by calculating the weighted mean from the grains of a partially-bleached population that were well bleached upon deposition (Thomsen et al., 2007). The *calc_IEU* function is easy to use and rapidly automates the calculations. In addition to calculating the IEU D_e value, the function uses fixed values of *Dbar* across a range of the D_e distribution to assess whether there is more than one solution for the model using the specified parameters. The efficiency of the *calc_IEU* function in calculating the IEU D_e value for a dataset means that sensitivity tests of the model to changing input parameters can be rapidly assessed. The sensitivity of the IEU D_e value to varying the amount of uncertainty arising from the scatter in a naturally well-bleached D_e distribution (i.e. the *a* value) has been investigated for the example dataset in this study. The results demonstrate that the IEU D_e value for these data is highly sensitive to the value of a used. Performing sensitivity tests of the IEU D_e value to parameters (e.g. a) can be particularly useful for luminescence dating of samples that are potentially complicated by additional sources of extrinsic uncertainty that are difficult to quantify (e.g. microdosimetry or bioturbation).

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Reviewer

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