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On the intrinsic accuracy and precision of the standardised growth curve (SGC) and global-SGC (gSGC) methods for equivalent dose determination: A simulation study

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HIGHLIGHTS

- Standardised growth curve (SGC) method is efficient procedure during luminescence dating.
- Recent global standardised growth curve (gSGC) method is improved SGC procedure.
- Simulations are performed of intrinsic accuracy and precision of SGC and gSGC.
- gSGC is intrinsically more precise than SGC method and more accurate for doses >210 Gy.

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ABSTRACT

In optically stimulated luminescence (OSL) dating, the single aliquot regenerative-dose (SAR) method has been used extensively for determining equivalent doses (D_e) in quartz. A variation of the SAR method is the "standardised growth curve" (SGC) method, which has been used as an efficient procedure to save measurement time during dating studies. During the application of the SGC method one establishes the SGC and calculation of the D_e of an aliquot requires only measurement of the standardised natural dose signal. Recently, a "global standardised growth curve" (gSGC) method was developed as an improved version of the SGC procedure. During the application of the gSGC method, the growth curves are re-normalised using sensitivity-corrected signal corresponding to one of the regenerative doses. Subsequently the D_e of an aliquot is estimated using the sensitivity-corrected natural dose signal and an additional sensitivity-corrected regenerative dose signal as well as the established gSGC. In the present study, simulations are performed to assess the intrinsic accuracy and precision of the SGC and gSGC D_e estimates. The results of our simulations validate that the gSGC method is intrinsically more precise than the SGC method and is also more accurate for doses greater than 210 Gy. Several factors which affect the reliability of the two methods are investigated.

1. Introduction

Luminescence dating techniques are well-established experimental methods for determining the absorbed total cumulative dose from natural radiation sources for archaeological and geological samples (Aitken, 1998; Wintle, 2008). The single aliquot regenerative-dose (SAR) protocol (Murray and Wintle, 2000) used in optically stimulated luminescence (OSL) dating is one of the most widely used dating techniques and has been successfully applied to quartz grains from a wide variety of Quaternary sediments (Murray and Olley, 2002). During the application of the SAR method, the sensitivity-corrected natural dose signal is projected onto the growth curve that is constructed using a series of sensitivity-corrected regenerative dose signals, in order to calculate the corresponding equivalent dose (D_e). The "standardised growth curve" (SGC) procedure (Roberts and Duller, 2004) has been frequently applied in combination with the SAR protocol to speed

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Table 1
Simulation steps used to generate the sensitivity-corrected natural dose signal L_n/T_n and an additional sensitivity-corrected regenerative dose signal L_r/T_r.

1 Natural quartz sample: Set all trap populations to zero
2 Geological dose: 1000 Gy at 1 Gy s^{-1} at 20 °C
3 Geological time: Heat to 350 °C
4 Repeated daylight exposures over long time: Illuminate for 100 s at 200 °C
5 Burial dose: 20 Gy at 220 °C at 0.01 Gy s^{-1}
6 Laboratory bleaching: Optical stimulation at 125 °C for 100 s
7 Give laboratory dose: $\mathbf{D_n}$ Gy at 1 Gy s^{-1} at 20 °C
8 Preheat to 260 °C for 10 s
9 Optical stimulation at 125 °C for 100 s (record $\mathbf{L_n}$)
10 Give test dose $\mathbf{D_t} = 0.1\mathbf{D_n}$ Gy at 1 Gy s^{-1} at 20 °C
11 Preheat to 220 °C for 10 s
12 Optical stimulation at 125 °C for 100 s (record $\mathbf{T_n}$)
13 Give regenerative dose: $\mathbf{D_r}$ Gy at 1 Gy s^{-1} at 20 °C ($\mathbf{D_r} = 0.8\mathbf{D_n}$)
14 Preheat to 260 °C for 10 s
15 Optical stimulation at 125 °C for 100 s (record $\mathbf{L_r}$)
16 Give test dose $\mathbf{D_t} = 0.1\mathbf{D_n}$ Gy at 1 Gy s^{-1} at 20 °C
17 Preheat to 220 °C for 10 s
18 Optical stimulation at 125 °C for 100 s (record $\mathbf{T_r}$)

Table 2
Simulation steps used to generate a series of sensitivity-corrected regenerative dose signals L_{ri}/T_{ri} to construct random growth curves.

1–5 Steps 1–5 are the same as in Table 1
6 Laboratory bleaching: Optical stimulation at 125 °C for 100 s
7 Irradiate sample with regenerative dose $\mathbf{D_{ri}}$ (for i = 1,2,3,4,5)
($\mathbf{D_{r1}} = 0.01\mathbf{D_n}$, $\mathbf{D_{r2}} = 0.4\mathbf{D_n}$, $\mathbf{D_{r3}} = 0.8\mathbf{D_n}$, $\mathbf{D_{r4}} = 1.2\mathbf{D_n}$, $\mathbf{D_{r5}} = 1.6\mathbf{D_n}$)
8 Preheat to 260 °C for 10 s
9 Optical stimulation at 125 °C for 100 s (record $\mathbf{L_{ri}}$)
10 Give test dose $\mathbf{D_t} = 0.1\mathbf{D_n}$ Gy at 1 Gy s^{-1} at 20 °C
11 Preheat to 220 °C for 10 s
12 Optical stimulation at 125 °C for 100 s (record $\mathbf{T_{ri}}$)
13 Repeat steps 7–12 with a subsequent regenerative dose $\mathbf{D_{ri}}$

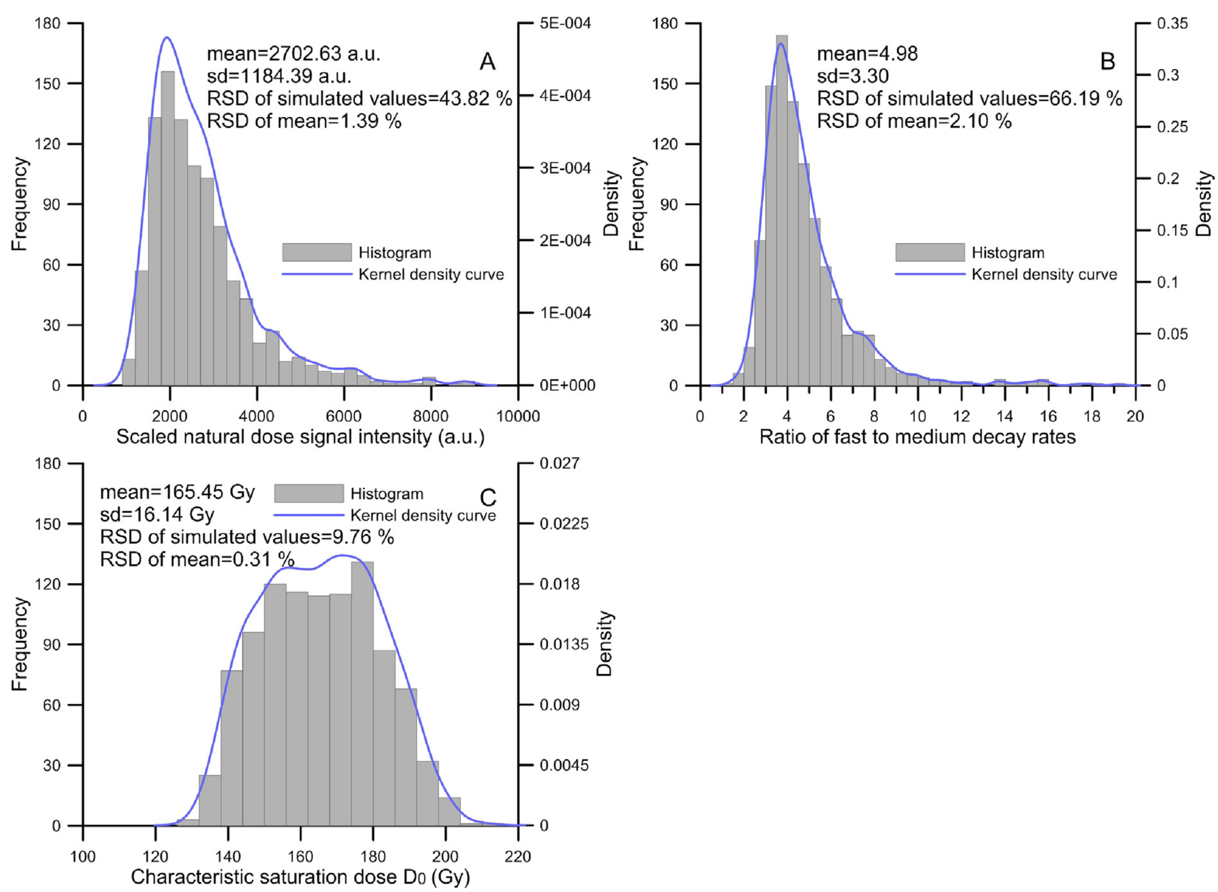

Fig. 1. Histograms and kernel density curves for simulated natural dose signal intensity (A), ratio of fast to medium decay rates (B), and characteristic saturation dose D_0 (C) for a given dose of 240 Gy. The number of simulations was 1000.

up the measurement process during D_e determination. Roberts and Duller (2004) firstly applied the SGC method to coarse-grained quartz from Tasmania and fine polymineral grains of loess from China, and found that a universal SGC exists for samples from different continents. Lai (2006) used the SGC procedure to determine D_e values of silt-sized quartz extracted from loess samples from the Chinese Loess Plateau, and concluded that a common growth curve exists for samples younger than approximately 270 ka.

Stevens et al. (2007) tested the validity of the SGC method using quartz grains obtained from samples of Chinese loess; they suggested that the SGC approach is particularly suited to high-resolution sampling studies of loess deposition, in which large numbers of samples from the same sections are analyzed. Long et al. (2010) investigated the applicability of the SGC procedure for estimating D_e values of lacustrine sediments from the Qaidam Basin of the Qinghai-Tibetan Plateau in China, and they showed that D_e values determined by the SGC approach are in agreement with those calculated based on a full SAR protocol for lacustrine samples, for dose values up to approximately 400 Gy. Yang et al. (2011) applied the SGC method to aeolian samples collected from sand fields in northeastern China, and found that the ratio of SAR D_e to SGC D_e values fall within ± 10% of each other, for D_e values smaller than approximately 50 Gy.

Burbidge et al. (2006) measured quartz samples from the Old Scatness Broch and Sumburgh Hotel Gardens sites using a refined SGC method. In their experiments an extra regenerative dose point close to the expected D_e value of each sample was used. In this way the regenerative dose predicted using the SGC can be compared with the extra regenerative dose given to each sample. This

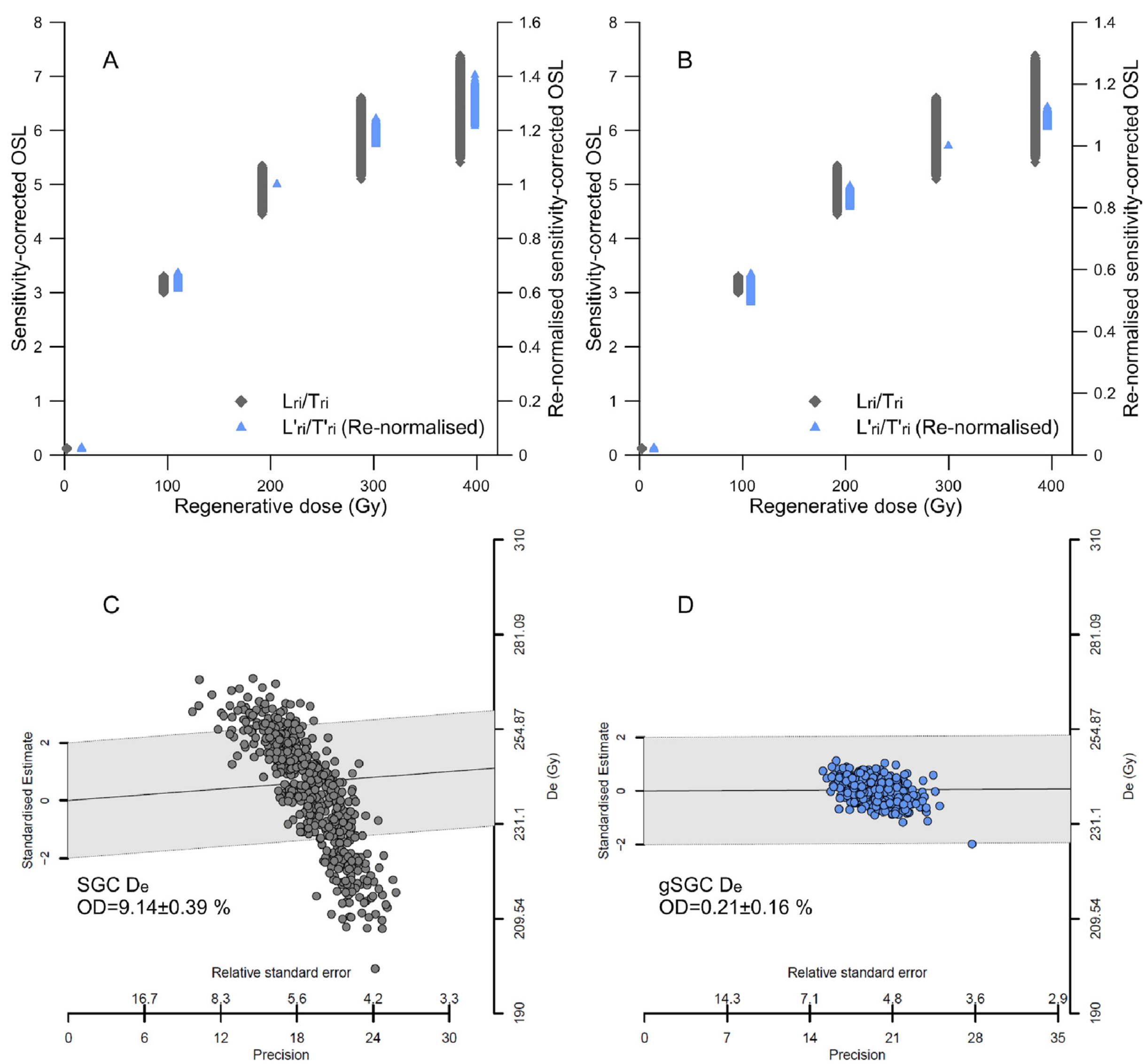

Fig. 2. (A) and (B) show the simulated sensitivity-corrected regenerative dose signals L_{ri}/T_{ri} (grey points) from 3000 random growth curves and their re-normalised counterpart L'_{ri}/T'_{ri} (blue points) for a given dose $D_n = 240$ Gy. The five regenerative dose points used for growth curve construction are 2.4, 96, 192, 288, and 384 Gy. L'_{ri}/T'_{ri} values in (A) and (B) are re-normalised using the third (i.e., $L'_{ri}/T'_{ri} = [L_{ri}/T_{ri}]/[L_{r3}/T_{r3}]$) and fourth (i.e., $L'_{ri}/T'_{ri} = [L_{ri}/T_{ri}]/[L_{r4}/T_{r4}]$) regenerative doses, respectively. It should be noted that the SGC is normally plotted as sensitivity-corrected regenerative dose signal multiplied by test dose (i.e., $[L_{ri}/T_{ri}] \times D_t$) but the multiplication is not necessary internally within this study because the same test dose magnitude was used for growth curves simulated for the same given dose. Note that the re-normalised data are offset by a few Gy to the right on the x-axis for clarity. (C) and (D) show pseudo radial plots of simulated 500 D_e values obtained from the SGC and gSGC methods respectively, for a given dose of 240 Gy. The gSGC D_e values demonstrated in (D) were calculated using randomly simulated re-normalised sensitivity-corrected regenerative dose signals shown in (B). OD denotes the calculated over-dispersion using the central age model of Galbraith et al. (1999). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

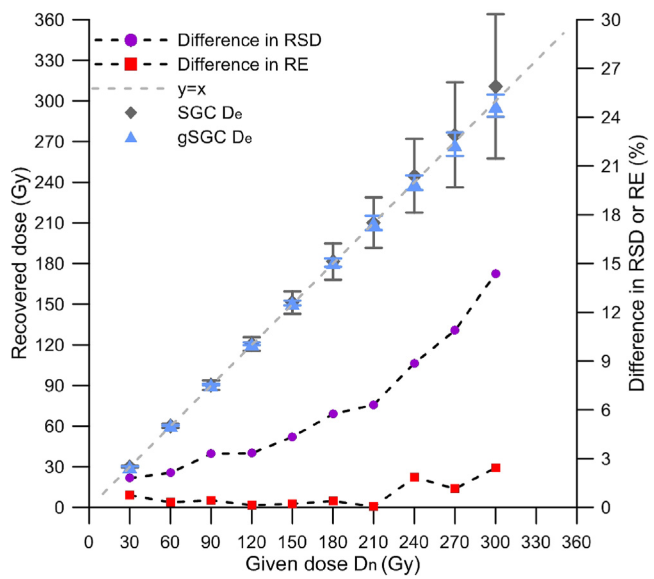

Fig. 3. The results of the SGC and gSGC simulations for given doses D_n in the range 30–300 Gy. The average doses were calculated using 500 versions of random parameters. The error bars denote the standard deviation of the 500 model variants. RSD and RE differences between the SGC and gSGC D_e estimates were indicated by purple circle and red rectangle, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

provides a check on the applicability of the SGC method employed. Telfer et al. (2008) tested the performance of the SGC method using samples from a range of environments in southern Africa and Florida. They found significant D_e underestimation when using the SGC to determine D_e values for a sample from Florida, which did not show regenerative growth characteristics in accordance with any other samples. They advocated the use of regionally based SGC for full D_e determination, and reiterated the recommendation of Burbidge et al. (2006) to incorporate a single regenerative step in the SGC procedure, so as to check for consistency. Similarly, Shen and Mauz (2011) estimated D_e values of late Pleistocene fine silt quartz from the Lower Mississippi Valley using the SGC method, and used the OSL response of a regenerative dose comparable in size to the expected dose to assess the reliability of D_e estimates derived from the SGC method.

Recently, Li et al. (2015a, 2015b) proposed a method to reduce the effect of between-aliquot variation in growth curves, by normalising the growth curves using sensitivity-corrected signal corresponding to one of the regenerative doses; they referred to this procedure as “re-normalisation”. The re-normalisation method requires the measurement of an extra sensitivity-corrected regenerative dose signal, in addition to the sensitivity-corrected natural dose signal. Li et al. (2015a) found a common re-normalised dose response curve which extended to doses of approximately 250 Gy for quartz samples with different geological provenances, sedimentary contexts and depositional ages. Their study indicated the possibility of developing a “global standardised growth curve” (gSGC) for the OSL signals from single aliquots of quartz.

The purpose of this paper is to simulate dose recovery experiments for the SGC and gSGC procedures, in order to assess the intrinsic accuracy and precision of SGC and gSGC D_e estimates. The simulations are carried out using the comprehensive kinetic model for quartz developed by Bailey (2001). Several factors that can potentially affect the reliability of the methods are investigated. To the best of our knowledge, there are no published simulation studies of these methods using kinetic models.

We investigated the relative error (RE) and relative standard deviation (RSD) of SGC and gSGC D_e estimates by simulating random variations of the concentrations of electrons and holes in the model, and also by random variation of the decay constants of the fast and medium decaying components in the OSL signal. The procedure simulates a dose recovery test, where an optically bleached “natural” quartz sample was irradiated with a laboratory dose in the range 30–300 Gy, and finally the given dose was recovered using the SGC and gSGC methods. The percentage difference between the given dose and the recovered dose denotes the RE of the methods. A Gaussian probability function was applied to the simulated D_e values to estimate the RSD of the methods.

It should be noted that uncertainties in the D_e values simulated in the present study are of a random rather than a systematic nature, and that the overall accuracy and precision of the methods will have contributions from several other factors such as photon counting statistics (Galbraith, 2002; Li, 2007; Adamiec et al., 2012; Bluszcz et al., 2015) and instrument reproducibility (Truscott et al., 2000; Thomsen et al., 2005; Jacobs et al., 2006; Duller, 2008), which are beyond the subject of this paper.

2. Simulation of dose recovery experiments to determine SGC and gSGC D_e estimates

In this paper random variations in quartz samples were simulated using a Monte Carlo method, as described in detail in previous studies (Bailey, 2004; Pagonis et al., 2011a, 2011b, 2011c). The model developed by Bailey (2001) consists of five electron traps and four hole centers and is able to reliably reproduce a wide variety of TL and OSL phenomena in quartz (Bailey, 2001; Pagonis et al., 2007a, 2007b, 2008). Levels 3 and 4 in this model (usually termed the fast and medium OSL components) yield TL peaks at approximately 330 °C and give rise also to OSL signals. The OSL signals from levels 3 and 4 are most suitable for the SAR protocol, and are of particular relevance in the simulation experiments described in this paper.

The experimentally observed variability in OSL characteristics of quartz grains was simulated by allowing trap concentrations to vary randomly within ± 20% of the original values, using uniformly distributed random numbers. The simulations also incorporated the experimentally observed large variations of the decay constants for the fast and medium components in a quartz sample. These variations were simulated using two Gaussian distributions based on the experimental values of the decay constants obtained by Feathers and Pagonis (2015). The average decay constant of $10.3 \pm 3.4\ s^{-1}$ was used for the fast component, and a value of $2.1 \pm 0.7\ s^{-1}$ for the medium component. These values are comparable to those obtained by Duller (2012), namely $11.1 \pm 4.3\ s^{-1}$ and $1.94 \pm 1.0\ s^{-1}$, respectively.

The dose recovery experiments used for determining the SGC and gSGC D_e were simulated using the open source R program KMS (Peng and Pagonis, 2016). SGC and gSGC D_e values were calculated using the function calED() from the R package numOSL (Peng et al., 2013). The procedure used in the dose recovery simulations of SGC and gSGC methods in this paper consists of two independent parts, as summarized in Table 1 and Table 2.

In the dose recovery simulations, the burial dose (Table 1 step 5) was optically bleached in the laboratory (Table 1 step 6) and irradiated with a dose D_n (Table 1 step 7) in the range 30–300 Gy. This given dose was treated as the “natural” dose to be determined using the SGC and gSGC methods. The test dose D_t was set equal to $0.1D_n$ (Table 1 step 10).

Steps 1–5 of Table 1 are used for simulating the geological history for the quartz sample, as proposed by Bailey (2001). Steps 6–12 of Table 1 are used to simulate the sensitivity-corrected given (natural) dose signal L_n/T_n used for calculating the SGC D_e. Steps 13–18 of Table 1 simulate the additional sensitivity-corrected regenerative dose signal L_r/T_r required to determine the gSGC D_e. The same L_n/T_n values were used for both SGC and gSGC D_e determination with the difference being in the gSGC method the L_n/T_n values were re-normalised with an additional D_r (L_r/T_r), whereas in the SGC method the L_n/T_n values remained un-normalised. Table 2 lists the steps for simulating a series of sensitivity-corrected regenerative dose signals L_{ri}/T_{ri}, which are used to construct the growth curves required by the SGC and gSGC methods. Note that regenerative doses D_{ri} used to construct a growth curve were measured on a single aliquot rather than on different aliquots. There are some additional steps in the simulations which are not shown explicitly in Tables 1 and 2. Specifically after each excitation stage in the simulations a relaxation period is introduced in order to allow the concentrations of electrons in the conduction band and holes in the valence band to decay to negligible values (Pagonis et al., 2006). After each heating step the model

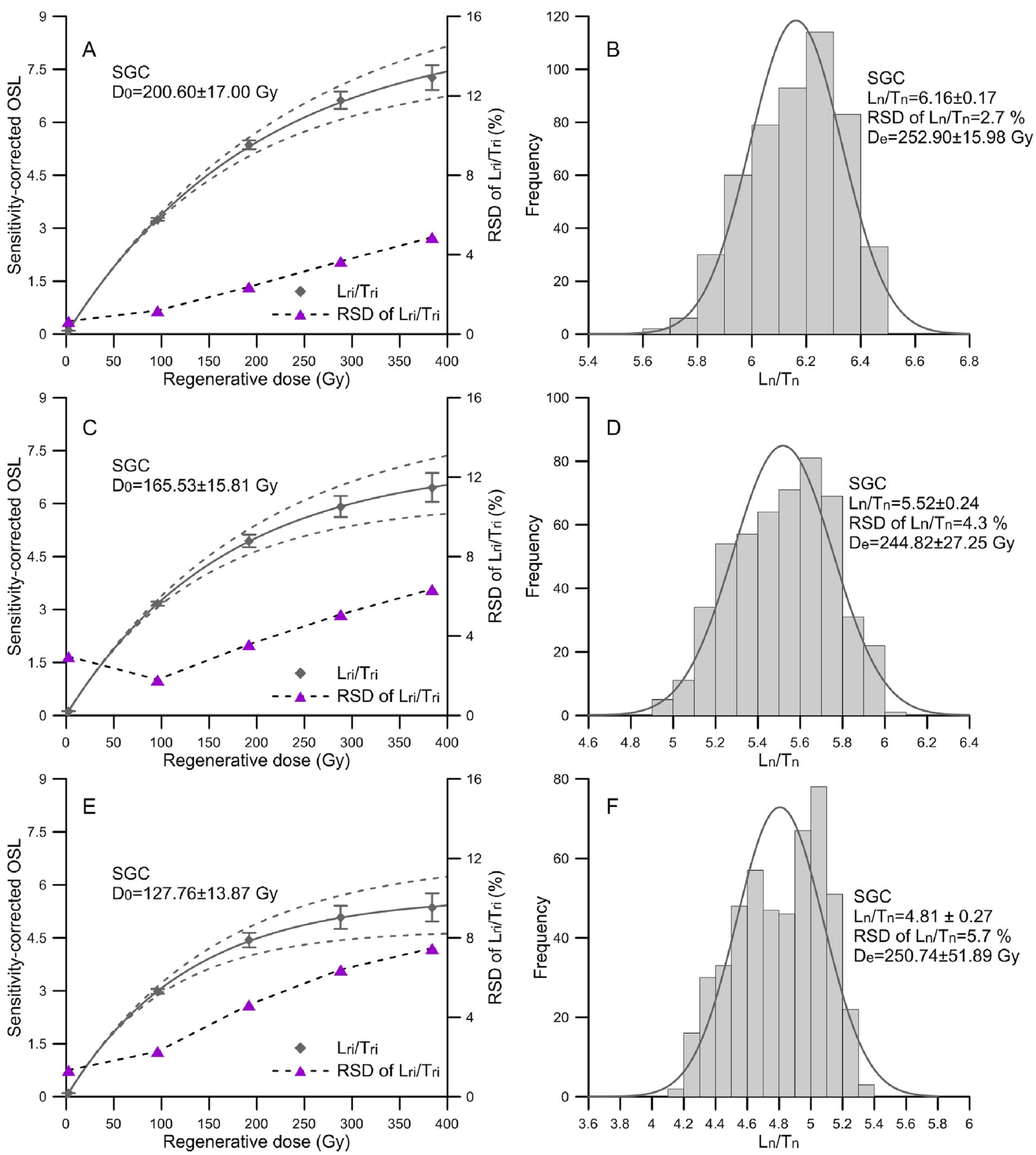

Fig. 4. (A), (C), and (E) are the result of averaging 3000 simulated random growth curves for a given dose $D_n = 240$ Gy, using N_8 values of 1×10^6, 1×10^{11}, and 1×10^{16} cm^{-3}, respectively. The regenerative dose points used to construct the growth curves are 2.4, 96, 192, 288, and 384 Gy. Two additional growth curves indicated by dashed lines denote the 95% confidence limits of the simulated L_{ri}/T_{ri} values. (B), (D), and (F) are the distributions of 500 simulated sensitivity-corrected given (natural) dose signal L_n/T_n for a given dose of 240 Gy, using N_8 values of 1×10^6, 1×10^{11}, and 1×10^{16} cm^{-3}, respectively. The resulting distributions of the 500 L_n/T_n values were fitted with Gaussian distributions, as indicated by the grey lines.

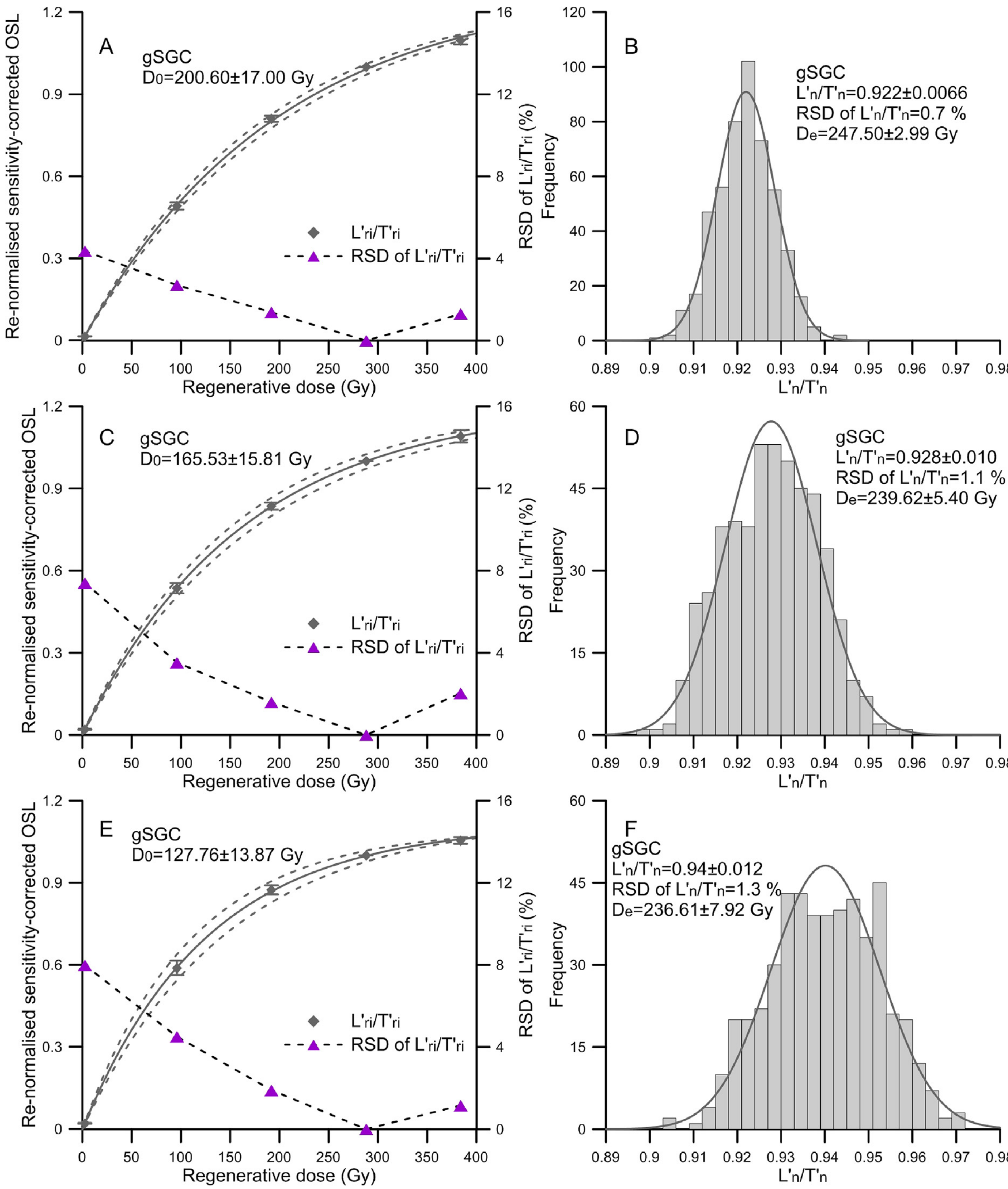

Fig. 5. The same data as in Fig. 4. (A), (C) and (E) were re-normalised using the fourth regenerative dose D_{r4} (L_{r4}/T_{r4}) (i.e., $L'_{ri}/T'_{ri} = [L_{ri}/T_{ri}]/[L_{r4}/T_{r4}]$). (B), (D), and (F) show the distributions of re-normalised sensitivity-corrected given (natural) dose signal L'_n/T'_n.

simulates a cooling-down period with a constant cooling rate of $-5\,^{\circ}\mathrm{C\,s^{-1}}$. Readers are referred to the paper by Peng and Pagonis (2016) for details of these additional steps used in the simulations.

Each random growth curve is constructed using five regenerative dose points D_{ri} (Table 2), which are chosen in such a way that the resultant sensitivity-corrected regenerative dose signals L_{ri}/T_{ri} encompass the sensitivity-corrected given (natural) dose signal L_n/T_n. Sensitivity-corrected given (natural) dose and additional regenerative dose signals were used in combination with randomly simulated growth curves, to determine the SGC and gSGC D_e values. The specific details of these steps are presented in the next section.

In this paper, unless otherwise stated, the simulations were repeated using 500 randomly generated versions of parameters for each given dose point, and 6 aliquots (growth curves) were used to construct the average dose response curve (re-normalised dose response curve) for determination of the SGC (gSGC) D_e values. During simulation of the gSGC D_e values, unless otherwise stated, the fourth regenerative dose D_{r4} (L_{r4}/T_{r4}) was used to re-normalise