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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.

Keywords

curve, growth, intrinsic, accuracy, study, simulation, determination, precision, dose, standardised, equivalent, methods, gsgc, global, sgc

Disciplines

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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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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.

Keywords: Standardised growth curve, equivalent dose, kinetic simulation, re-normalisation

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 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 $\pm 10\%$ 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 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 $10.3 \pm 3.4 \text{ s}^{-1}$ was used for the fast component, and a value of $2.1 \pm 0.7 \text{ s}^{-1}$ for the medium component. These values are comparable to those obtained by Duller (2012), namely $11.1 \pm 4.3 \text{ s}^{-1}$ and $1.94 \pm 1.0 \text{ s}^{-1}$, 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 `calLED()` from the R package numOSL (Peng et al., 2013). 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). The procedure used for determining the “natural” dose using SGC and gSGC methods consists of two independent parts, as summarized in Table 1 and Table 2.

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 simulates a cooling-down period with a constant cooling rate of $-5 \text{ }^\circ\text{C s}^{-1}$. 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 the growth curves (i.e., $L'_{ri}/T'_{ri}=[L_{ri}/T_{ri}]/[L_{r4}/T_{r4}]$, where L'_{ri}/T'_{ri} denotes the re-normalised sensitivity-corrected regenerative dose signals), and the additional regenerative dose D_r required for determining the gSGC D_e was set equal to $0.8D_n$. The average dose response curve (re-normalised dose response curve) was fitted using a single saturating exponential function in order to calculate the SGC (gSGC) D_e .

We obtained decay rates for the fast and medium components by deconvoluting simulated decay curves into two first-order exponential decaying components as well as a constant component using the `decomp()` function from the R package numOSL. We obtained the characteristic saturation dose D_0 values by fitting the growth curves with the single saturating exponential model using the `fitGrowth()` function from the R package numOSL. The resultant variations in simulated natural dose signal intensity, ratio of fast to medium decay rates, and characteristic saturation dose D_0 were demonstrated in Fig. 1A, B, and C, respectively, for a given dose of 240 Gy. The % variations of these parameters are generally within the ranges of typical experimental OSL data.

Fig. 2A and B show the sensitivity-corrected regenerative dose signals L_{ri}/T_{ri} and their re-normalised counterpart L'_{ri}/T'_{ri} correspondingly, for 3000 randomly simulated growth curves for a given dose of 240 Gy. These figures demonstrate that the re-normalisation procedure used in the gSGC procedure can reduce significantly the scatter of the sensitivity-corrected regenerative dose signals. Specifically, if we denote the fifth sensitivity-corrected regenerative dose signal before

and after re-normalisation as L_{r5}/T_{r5} and L'_{r5}/T'_{r5} , respectively, then the RSD in L_{r5}/T_{r5} is 6.18 %. The RSD for L'_{r5}/T'_{r5} reduces to 2.73 % if the third regenerative dose D_{r3} (L_{r3}/T_{r3}) is used to re-normalise the growth curve (i.e., $L'_{ri}/T'_{ri}=[L_{ri}/T_{ri}]/[L_{r3}/T_{r3}]$) (Fig. 2A). The RSD for L'_{r5}/T'_{r5} is further reduced to 1.15 % if the fourth regenerative dose D_{r4} (L_{r4}/T_{r4}) is used for re-normalisation (i.e., $L'_{ri}/T'_{ri}=[L_{ri}/T_{ri}]/[L_{r4}/T_{r4}]$) (Fig. 2B).

Fig. 2C and D show the simulated D_e distributions obtained from the SGC and gSGC methods respectively, for a given dose of 240 Gy, visualized by a simplified (pseudo) radial plot (Galbraith, 1988) implemented using function `psRadialPlot()` from the R package `numOSL`. The recovered average D_e values using the SGC and gSGC methods are 244.82 Gy and 239.62 Gy respectively. The standard deviations of the 500 model variants calculated from the SGC and gSGC methods are 27.25 Gy and 5.40 Gy respectively. Accordingly, the RSD for the SGC and gSGC D_e estimates are 11.13 % and 2.25 %, respectively. The over-dispersion values (Galbraith et al., 1999) for the recovered SGC and gSGC D_e distributions are 9.14 ± 0.39 % and 0.21 ± 0.16 % respectively. These simulation results suggest that the gSGC method can greatly improve the precision of D_e estimates over the SGC method.

Fig. 3 shows a comparison of recovered D_e estimates obtained by the SGC and gSGC methods for given doses D_n in the range 30–300 Gy. It can be observed from Fig. 3 that for given doses less than 120 Gy the differences in RSD and RE between SGC and gSGC D_e values are smaller than 4 %. The difference in RSD between D_e estimates obtained from the two methods increases substantially when the given dose exceeds 120 Gy. However, the overall differences in RE are smaller than 3 % for investigated dose values up to 300 Gy. The simulation indicates that the gSGC method can significantly improve the precision of D_e estimates compared to the SGC method, though the difference in accuracy between D_e estimates obtained from the two methods is not very significant for given dose less than 210 Gy.

3. Investigation of factors influencing the reliability of the SGC and gSGC D_e estimates

In this section, we investigate the effect of various parameters on the reliability of the SGC and gSGC D_e estimates; these parameters are the characteristic saturation dose D_0 of a growth curve, the number of aliquots used for SGC and gSGC establishment, the size of the additional regenerative dose D_r (L_r/T_r) used for re-normalising the sensitivity-corrected natural dose signal,

and the size of the regenerative dose D_{ri} (L_{ri}/T_{ri}) used for re-normalising the growth curves. It deserves to point out that it is not always the case that the sensitivity-corrected natural dose signal and the growth curves should be re-normalised by regenerative dose of the same magnitude (i.e., D_r may not be equal to D_{ri}) during gSGC D_e estimation. A researcher may use an additional regenerative dose D_r that is different in magnitude from all of the D_{ri} values but close in size to the given dose D_n for re-normalising the sensitivity-corrected natural dose signal in order to improve the precision of calculated gSGC D_e .

We simulated the dose recovery experiments using different values for the kinetic parameter N_8 (i.e., the total concentration of holes for the “luminescence center” L), in order to change the characteristic saturation dose D_0 of the generated random growth curves. It was found in the simulations that as the value of the parameter N_8 is increased in the model, the sensitivity of the simulated signals will also increase. Specifically larger values of N_8 yield greater signal intensity for both the regenerative dose OSL response L_{ri} and for the test dose OSL response T_{ri} . Furthermore, simulated L_{ri} and T_{ri} with greater signal intensity result in simulated growth curves which tend to saturate at lower doses. Consequently, a larger N_8 value results in smaller D_0 values for the growth curves, and vice versa.

Fig. 4 illustrates random growth curves and sensitivity-corrected given (natural) dose signals simulated using the SGC method. Fig. 4A, C, and E show respectively distributions of 3000 variants of random growth curves simulated using N_8 values of 1×10^6 , 1×10^{11} , and $1 \times 10^{16} \text{ cm}^{-3}$ for a given dose $D_n=240 \text{ Gy}$. The corresponding characteristic saturating dose D_0 are $200.60 \pm 17.00 \text{ Gy}$, $165.53 \pm 15.81 \text{ Gy}$, and $127.76 \pm 13.87 \text{ Gy}$, respectively. It suggests that the variability in growth curves is insignificant for regenerative dose below 100 Gy, and it increases substantially with increase in regenerative dose afterwards. This also implies that the observed larger uncertainty in SGC D_e estimates of Fig. 3 is mainly caused by the large variability of growth curves for regenerative dose above 100 Gy; it is concluded that the SGC method cannot effectively eliminate the between-aliquot scatter of different growth curves.

Fig. 4B, D, and F illustrate the effect of D_0 values on the distributions of sensitivity-corrected given (natural) dose signal L_n/T_n . The RSD of L_n/T_n for low, intermediate and high N_8 values are 2.7 %, 4.3 %, and 5.7 % respectively, suggesting that the variability of L_n/T_n increases as the D_0 values decrease. The uncertainty of resultant SGC D_e estimates also increases as D_0 decreases.

These results are consistent with Fig. 4A, C, and E, which demonstrates that the RSD of sensitivity-corrected regenerative dose signals L_{ri}/T_{ri} increases as D_0 decreases.

Fig. 5 shows the same data as in Fig. 4 (the data was re-normalised using the gSGC method). In Fig. 5A, C, and E, the simulated growth curves were re-normalised using the fourth regenerative dose D_{r4} (L_{r4}/T_{r4}) (i.e., $L'_{ri}/T'_{ri}=[L_{ri}/T_{ri}]/[L_{r4}/T_{r4}]$). In Fig. 5B, D, and F, the simulated sensitivity-corrected given (natural) dose signal was re-normalised using an additional regenerative dose D_r (L_r/T_r) and the established gSGC according to Eq. (10) of Li et al. (2015a). We denote this re-normalised sensitivity-corrected natural dose signal by L'_n/T'_n . It can be seen from Fig. 5A, C, and E that D_0 values of the re-normalised growth curves are the same as those in Fig. 4A, C, and E, suggesting that the re-normalisation procedure will not affect the D_0 values of the growth curves.

It can be observed from contrasting Fig. 4 and Fig. 5 that the variability of growth curves decreased significantly after applying the re-normalisation procedure. The scatter in re-normalised growth curves is not only small for regenerative dose less than 100 Gy but also less significant for larger regenerative doses (Fig. 5), in comparison to that illustrated in Fig. 4. The RSD of L'_n/T'_n for low, intermediate, high N_8 values are 0.7 %, 1.1 %, and 1.3 % respectively. These values are significantly smaller than those obtained in Fig. 4 for their un-normalised counterparts. A comparison between Fig. 4 and Fig. 5 clearly illustrates why the uncertainty of D_e estimates obtained from the gSGC method is significantly smaller than the ones obtained from the SGC method. The gSGC method reduces the variation in growth curves, to a much greater extent than the SGC method.

Fig. 6 demonstrates the variation of RSD and RE of SGC and gSGC D_e estimates with the D_0 (N_8). It can be seen from the scales of the y-axes that generally both the RSD and RE of D_e estimates obtained from the gSGC method are smaller than their SGC counterpart (except the $D_n=120$ Gy case). There is no obvious correlation between the RE of SGC and gSGC D_e estimates and the characteristic saturation dose D_0 for various given doses. In most cases, the D_e estimates yield lower RE (smaller than 4 %) using moderate D_0 values corresponding to the default N_8 value of $1 \times 10^{11} \text{ cm}^{-3}$ used in the model of Bailey (2001). A monotonic decrease in the RSD of SGC and gSGC D_e estimates with increased D_0 values was observed in almost all cases. This is because both the scatter in sensitivity-corrected natural dose and regenerative dose signals (as well as their

re-normalised counterparts) decreases with the increase in D_0 values, as was illustrated in Fig. 4 and Fig. 5.

During the application of the SGC (gSGC) method, the SGC (gSGC) used for D_e determination is usually established from the average of a number of growth curves (re-normalised growth curves) from different aliquots. Fig. 7 demonstrates the variation of RSD and RE of SGC and gSGC D_e estimates with the number of aliquots used for SGC and gSGC establishment. It can be observed from Fig. 7 that increasing the number of aliquots improves the precision of SGC and gSGC D_e estimates. This is because of overall improvements of the statistics; the uncertainty of the average dose response curve (re-normalised dose response curve) used to determine the SGC (gSGC) D_e values will decrease by using more aliquots in the procedure.

Using more aliquots also improves the accuracy of SGC D_e estimates, as illustrated in Fig. 7A, C, and E. However, it seems that the accuracy of gSGC D_e estimates is not sensitive to the variation of number of aliquots, and shows a random variation pattern. This may imply that in the gSGC method the number of aliquots used for gSGC establishment is not a major factor controlling the accuracy of D_e estimates.

In most cases both the RSD and RE of D_e estimates obtained from the gSGC method are significantly smaller than their SGC counterpart. An exception is that the RE of gSGC D_e estimates is slightly larger than that obtained by the SGC method for a given dose $D_n=120$ Gy when the number of aliquots exceed 6, as demonstrated in Fig. 7A and B. This may suggest that when applying the gSGC method to determining D_e values smaller than 120 Gy, the gain in accuracy is not obvious compared to the SGC method. This is consistent with Fig. 3, which suggests that the difference in RE between the two methods is less than 1 % for given dose up to 210 Gy.

The re-normalisation procedure used in the gSGC method requires a sensitivity-corrected regenerative dose signal to be measured, in addition to the sensitivity-corrected natural dose signal. These signals are used in combination with the established gSGC in order to determine the gSGC D_e value. Fig. 8 plots the RSD and RE of gSGC D_e estimates against the size of the additional regenerative dose D_r . The results indicate that the size of the regenerative dose D_r (L_r/T_r) used for re-normalising the sensitivity-corrected natural dose signal can significantly affect the precision of gSGC D_e estimates (Fig. 8A). Recovered gSGC D_e values for different given doses are of low

RSD (smaller than 4 %), if the additional regenerative dose D_r varies between $0.8D_n$ and $1.2D_n$. The gSGC D_e estimates have the lowest RSD when the additional regenerative dose is set equal to the given dose (i.e., if $D_r=D_n$). The RSD of gSGC D_e estimates become increasingly larger with the increase in the difference between D_n and D_r . The simulation validates the conclusion drawn by Li et al. (2015a) that the chosen additional regenerative dose should be as close as possible in size to that of the natural dose, in order to minimize the scatter in the re-normalised sensitivity-corrected natural dose signal L'_n/T'_n .

However, there is no obvious correlation between the accuracy of gSGC D_e estimates and the size of the additional regenerative dose D_r (L_r/T_r) (Fig. 8B). In addition, the best accuracy of gSGC D_e estimates does not correspond to an additional regenerative dose that is equal in size to the given dose. Interestingly, for given dose $D_n=60$ Gy and $D_n=120$ Gy, gSGC D_e estimates have the lowest RE when the additional regenerative dose D_r is equal to $1.6D_n$. For given dose $D_n=240$ Gy and $D_n=300$ Gy, gSGC D_e estimates have the lowest RE when the additional regenerative doses are set equal to $0.6D_n$ and $0.4D_n$, respectively. This suggests that the correlation between accuracy of gSGC D_e estimates and the size of additional regenerative doses used for re-normalisation is complex, and does not follow a specific pattern. It seems that lower RE is obtainable when smaller additional regenerative dose is used for re-normalisation of a larger given dose, and vice versa.

Li et al. (2015a) illustrated how the choice of the size of the regenerative dose D_{ri} (L_{ri}/T_{ri}) used for re-normalising the growth curves affects the extent of variation between aliquots (growth curves). During the simulation it was observed that the scatter in re-normalised growth curves varies slightly when different regenerative doses D_{ri} (L_{ri}/T_{ri}) were used for re-normalisation of the growth curves, as demonstrated in Fig. 9 for a given dose of 240 Gy. The resultant mean RSD of L'_{ri}/T'_{ri} were 2.73 %, 2.31 %, 2.61 %, and 3.29 % respectively if regenerative dose values of $0.4D_n$, $0.8D_n$, $1.2D_n$, and $1.6D_n$ Gy were used for growth curve re-normalisation. Fig. 10 shows the influences of the size of the regenerative dose D_{ri} (L_{ri}/T_{ri}) used for re-normalising the growth curves on the RSD and RE of gSGC D_e estimates for different given doses. It can be observed from Fig. 10 that there is no obvious variation trend for the RSD or RE of gSGC D_e estimates with the regenerative dose D_{ri} (L_{ri}/T_{ri}) used for re-normalisation. It can be seen from the scales of y-axes in Fig. 10 that the influence of the regenerative dose sizes used for growth curve

re-normalisation on the RSD and RE of gSGC D_e estimates is relatively insignificant. For all the four investigated regenerative dose points, the variations in RSD and RE of gSGC D_e estimates are less than 0.1 %.

4. Conclusions

The comprehensive quartz model of Bailey (2001) was used in this paper to simulate dose recovery experiments to assess the intrinsic precision and accuracy of the SGC and gSGC D_e estimates. The simulation results show that the gSGC method can significantly improve the precision of D_e estimates compared to the SGC method. It suggests that the difference in RE between the SGC and gSGC methods is less than 3 % for investigated doses up to 300 Gy. However, the RSD of gSGC D_e estimates was significantly smaller than that of SGC D_e estimates. The simulation experiments validate that the between-aliquot scatter in growth curves can be effectively eliminated by using the re-normalisation procedure employed in the gSGC method.

Several factors which may be affecting both the intrinsic precision and the accuracy of the two methods were investigated. The simulation results suggest that:

(1) The precision of SGC and gSGC D_e estimates can be improved if growth curves with larger characteristic saturation dose D_0 are used.

(2) Using a larger number of aliquots (growth curves) to establish the SGC can improve both precision and accuracy of SGC D_e estimates. However, though the precision of gSGC D_e estimates also improves with the increase in the number of aliquots used for gSGC establishment, it seems that the accuracy of gSGC D_e estimates is not sensitivity to variation in number of aliquots.

(3) The precision of gSGC D_e estimates is very sensitive to the size of the additional regenerative dose D_r (L_r/T_r) used for re-normalising the sensitivity-corrected natural dose signal. Better precision is obtainable if the additional regenerative dose D_r used for re-normalisation is close in size to the given dose D_n .

(4) Both the precision and accuracy of gSGC D_e estimates are insensitive to the size of the regenerative dose D_{ri} (L_{ri}/T_{ri}) used for re-normalising the growth curves. For doses up to 300 Gy, the variations in RSD and RE of gSGC D_e estimates are less than 0.1 % when different regenerative dose sizes D_{ri} were used for re-normalisation.

The simulation results presented in this study demonstrate that the gSGC method is almost

always intrinsically more precise than the SGC method given that a proper size of additional regenerative dose D_r (L_r/T_r) is used for re-normalisation. Furthermore, although the difference in accuracy between the two methods is less significant for given doses less than 210 Gy, the gSGC method is obviously more accurate for larger doses. Therefore, we recommend use of gSGC method for future dating application if possible.

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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: 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 L_n)
10 Give test dose $D_t=0.1D_n$ 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 T_n)
13 Give regenerative dose: D_r Gy at 1 Gy s ⁻¹ at 20 °C ($D_r=0.8D_n$)
14 Preheat to 260 °C for 10 s
15 Optical stimulation at 125 °C for 100 s (record L_r)
16 Give test dose $D_t=0.1D_n$ 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 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 D_{ri} (for $i=1,2,3,4,5$) ($D_{r1}=0.01D_n$, $D_{r2}=0.4D_n$, $D_{r3}=0.8D_n$, $D_{r4}=1.2D_n$, $D_{r5}=1.6D_n$)
8 Preheat to 260 °C for 10 s
9 Optical stimulation at 125 °C for 100 s (record L_{ri})
10 Give test dose $D_t=0.1D_n$ 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 T_{ri})
13 Repeat steps 7–12 with a subsequent regenerative dose 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.

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. 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).

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.

Fig. 4. (A), (C), and (E) are the result of averaging 3000 simulated random growth curves for a given dose $D_n = 240 \text{ Gy}$, using N_8 values of 1×10^6 , 1×10^{11} , and $1 \times 10^{16} \text{ cm}^{-3}$, 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 $1 \times 10^{16} \text{ cm}^{-3}$, 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., $L'_n/T'_n = [L_{ri}/T_{ri}] / [L_{r4}/T_{r4}]$). (B), (D), and (F) show the distributions of re-normalised sensitivity-corrected given (natural) dose signal L'_n/T'_n .

Fig. 6. Variation of RSD and RE of SGC and gSGC D_e estimates with D_0 (N_8) for various given doses D_n . Each data point was based on 500 versions of simulation. The data points encircled by dashed circles denote the RE of D_e estimates simulated using the default N_8 value of $1 \times 10^{11} \text{ cm}^{-3}$.

Fig. 7. Variation of RSD and RE of SGC and gSGC D_e estimates with the number of aliquots used to establish the SGC and gSGC for various given doses D_n . The investigated number of aliquots ranges from 2 to 24 with an interval of 1. Each data point was based on 500 model variants.

Fig. 8. Variation of RSD (A) and RE (B) of gSGC D_e estimates with the size of the additional regenerative dose D_r (L_r/T_r) used to re-normalise the sensitivity-corrected natural dose signal for various given doses D_n . D_r ranges from $0.2D_n$ to $2D_n$ with a step of $0.2D_n$. Each data point was based on 500 model variants. Note that the scales of x-axes are expressed as percent of the given dose D_n .

Fig. 9. Variation of re-normalised sensitivity-corrected regenerative dose signals L'_{ri}/T'_{ri} with the size of regenerative dose D_{ri} (L_{ri}/T_{ri}) used for growth curve re-normalisation for a given dose of 240 Gy. (A), (B), (C), and (D) were re-normalised using regenerative dose values of $0.4D_n$, $0.8D_n$, $1.2D_n$, and $1.6D_n$ Gy (Table 2), respectively. Each subplot was based on 3000 randomly simulated growth curves.

Fig. 10. Variation of RSD and RE of gSGC D_e estimates with the size of the regenerative dose D_{ri} (L_{ri}/T_{ri}) used for growth curve re-normalisation for various given doses D_n . The four regenerative dose values used for re-normalisation are $0.4D_n$, $0.8D_n$, $1.2D_n$, and $1.6D_n$ Gy (Table 2). Each data point was based on 500 model variants. Note that the scales of x-axes are expressed as percent of the given dose D_n .