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Simulations of saturating exponential ESR/TL dose response curves - weighting of intensity values by inverse variance

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Introduction

This paper presents the continuation of numerical simulations that were presented by Grün and Rhodes (1991). These simulations were used to investigate the influence of various parameters (even/exponential dose distribution; maximum irradiation dose, D_{max}, precision of TL intensity, and number of data points) on the determination of the equivalent dose, D_E, and the associated error assuming equal weights for the ESR/TL intensity. It was concluded that the size of the D_E error is critically dependent on the precision of the measured ESR/TL intensity and also on the selection of the maximum irradiation dose and the dose step distribution. It was commented by Berger (1991) that the assumption of equal weights for the ESR/TL intensity may invalidate the derived conclusions. He suggested further tests for unequal weighting, specifically weighting by inverse variance. These simulations have been carried out and are presented in this contribution.

The technical and experimental procedures of this paper are identical to Grün & Rhodes (1991) to which the reader is referred. Parameters are defined as follows:

D_E	equivalent dose
D_0	characteristic saturation dose
D_{max}	maximum radiation dose
I	measured ESR/TL Intensity
I_{max}	maximum intensity when all traps are filled
s.d.	standard deviation of computed D_E distribution (random error)
dev.	deviation of mean value of D_E distribution from preset D_E (systematic error)
s.d.(I)	uncertainty of ESR/TL intensity

Two dose distribution models were investigated:

Model 1:	even dose spacing, (e.g. 0, 2, 4, 6, 8....)
Model 2:	doubling of an initial dose step (e.g. 0, 1, 2, 4, 8....).

Simulations were performed for various preset D_E/D_o ratios of 0.003, 0.015, 0.03, 0.15, 0.3 and 1.5 (for D_0 = 3333 Gy, these values correspond to dose values of 10, 50 100, 500, 1000 and 5000 Gy, respectively). The results in this paper are based on 2000 randomly generated sets of ESR/TL values.

Results

Effect of the maximum irradiation dose, D_{max}

As in the previous paper, this experiment is based on ten ESR/TL data points per dose response curve including the natural sample with an assumed uncertainty in the ESR/TL intensity of 2%.

Figure 1 shows the standard deviation (s.d.) in the determination of D_E and the systematic deviation of the computed mean D_E value from the preset D_E. In all cases where $D_E < D_0$ (fig. 1A-E, left), the error in D_E estimation decreases rapidly with increasing D_{max} values, reaching relatively low levels when $D_{max} \geq 10D_E$. Above a D_E/D_0 ratio of 0.15 (fig. 1D-F, left), the error in D_E becomes more critically dependent on the choice of D_{max}, because the plot of s.d.(D_E) versus D_{max}/D_E shows clear minima. In case $D_E > D_0$ (fig. 1F, left), the error in D_E determination is at least 20% for $D_{max} \approx 2\ D_E$.

In the range $D_E<0.03D_0$ systematic underestimations occur when $D_{max}<10D_E$ (fig. 1A-C, right), whereas in the D_E range from 0.15 to $0.3D_0$ systematic overestimations occur when using $D_{max}>10D_E$ (fig. 1D-F, right). A selection of $D_{max} \approx 10D_E$ leads to the smallest overall error (s.d. in D_E determination plus systematic error).

Effect of dose distribution model

The exponential dose distribution (model 2) resulted in somewhat smaller errors (5 to 15%) in D_E determination than the even dose distribution (model 1).

Effect of the precision of the ESR/TL intensity

Figure 2 shows the errors in D_E estimation for different uncertainties in the ESR/TL measurement (D_{max} = $10D_E$, except for $D_E = 1.5D_0$, here $D_{max} = 2D_E$). The uncertainty in D_E determination is strongly dependent on the intrinsic uncertainty of a ESR/TL measurement. A four-fold improvement in the precision reduces the error in D_E by a factor of about 3.5. D_E values close to saturation can be measured with a reasonable degree of confidence only if the precision of the ESR/TL measurement is better than 1%.

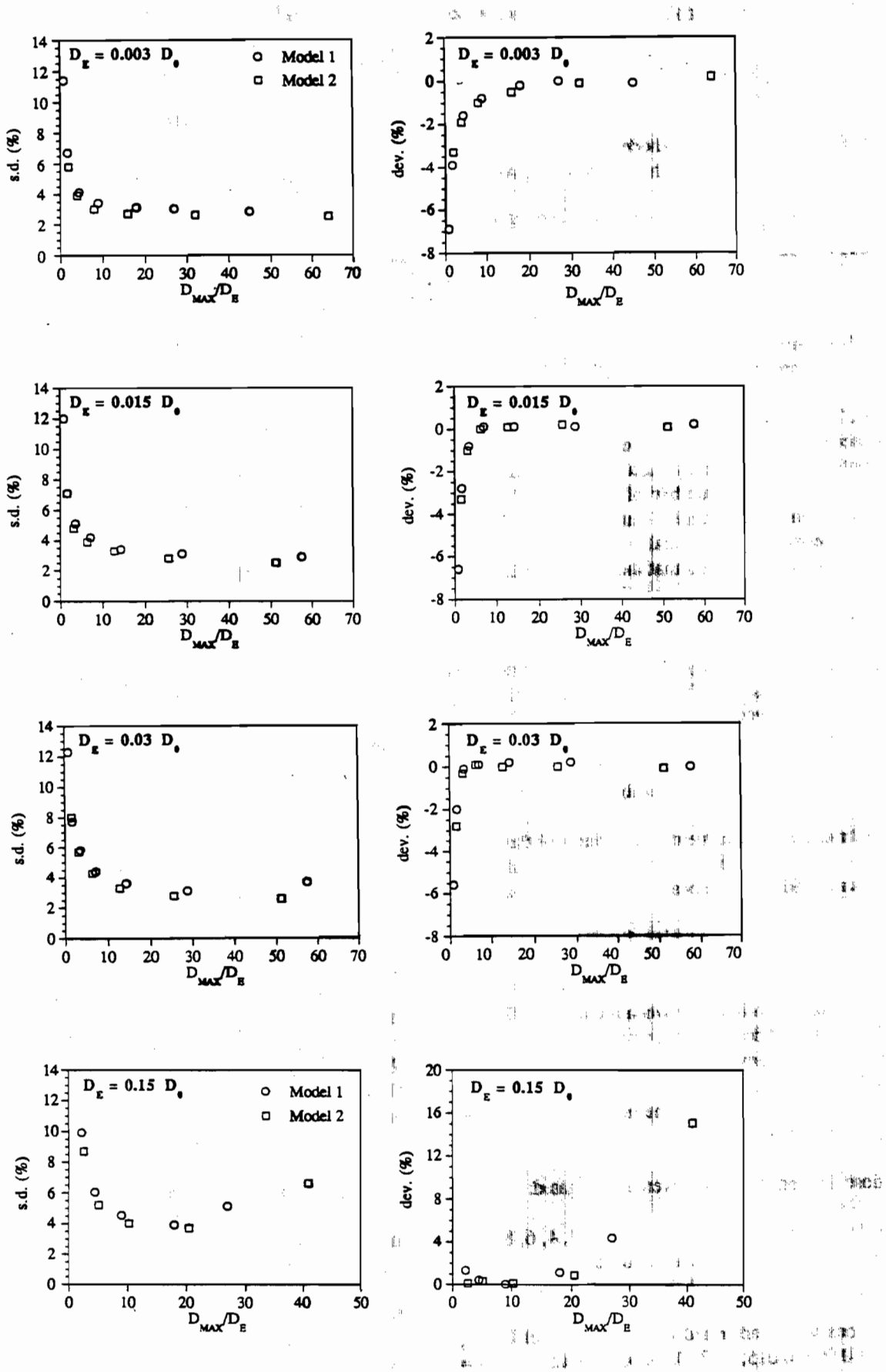

Figure 1. (A-D from top).
Standard deviation, s.d., (left) and systematic deviations (right) in D_E determination for preset D_E values of 0.003, 0.015, 0.03, 0.15, 0.3 and 1.5 D_0, 10 data points (one per dose) and a precision in ESR/TL intensity of 2%. Equal dose spacing (circles) and exponential dose spacing (squares).

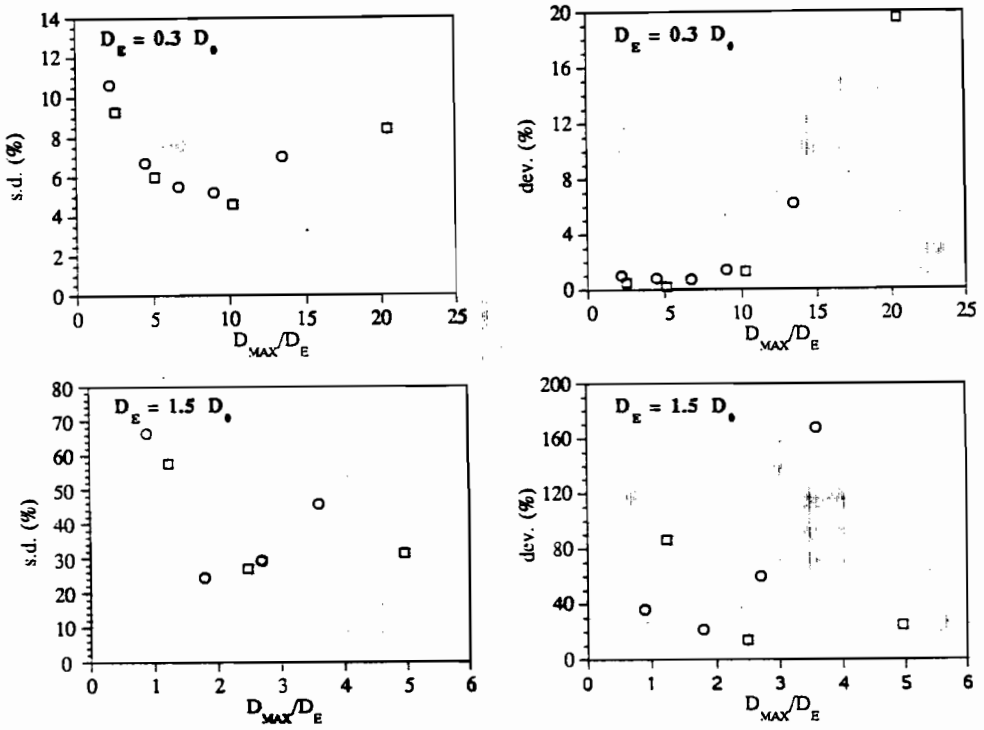

Figure 1. (E-F from top).
Standard deviation, s.d., (left) and systematic deviations (right) in D_E determination for preset D_E values of 0.003, 0.015, 0.03, 0.15, 0.3 and 1.5 D_0, 10 data points (one per dose) and a precision in ESR/TL intensity of 2%. Equal dose spacing (circles) and exponential dose spacing (squares).

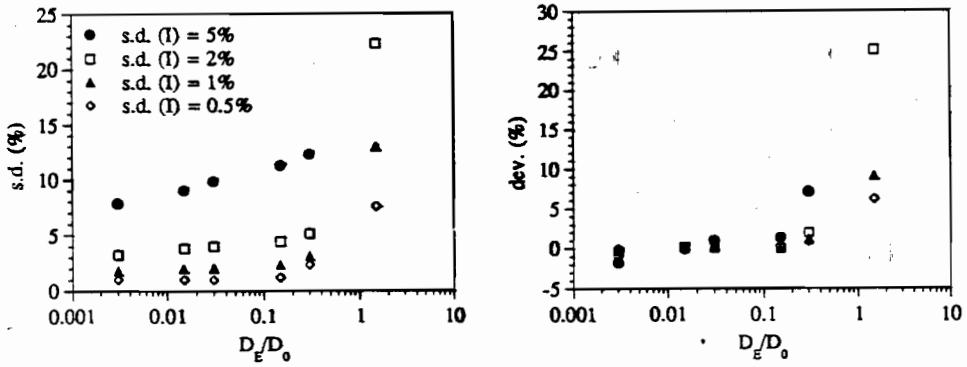

Figure 2.
Standard deviation, s.d., (left) and systematic deviations (right) in D_E determination for different precision in ESR/TL intensity, 10 data points, model 1 and $D_{max} = 10D_E$, except for $D_E = 1.5D_0$: $D_{max} = 2D_E$.

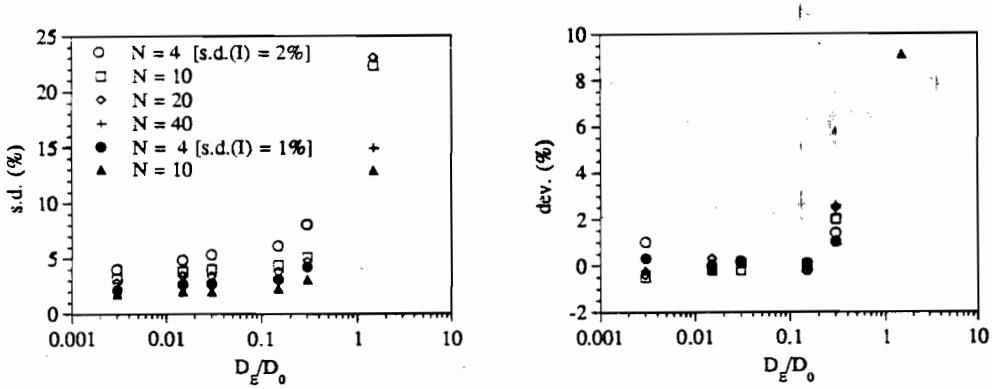

Figure 3.
Standard deviation, s.d., (left) and systematic deviations (right) in D_E determination for different number of data points, model 1 and $D_{max} = 10D_E$, except for $D_E = 1.5D_0$: $D_{max} = 2D_E$.

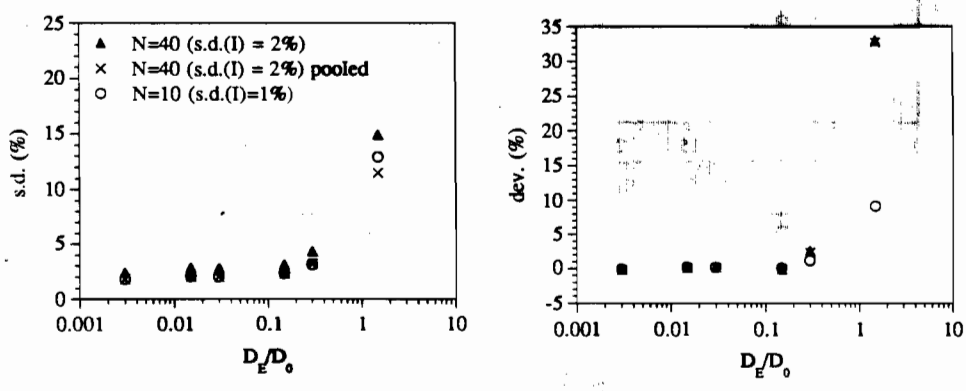

Figure 4.
Standard deviation, s.d., (left) and systematic deviations (right) in D_E determination for 40 data points, equally spaced and pooled at 10 equally spaced data points, respectively (2% precision), compared to 10 equally spaced data points with 1% precision. $D_{max} = 10D_E$, except for $D_E = 1.5D_0$: $D_{max} = 2D_E$.

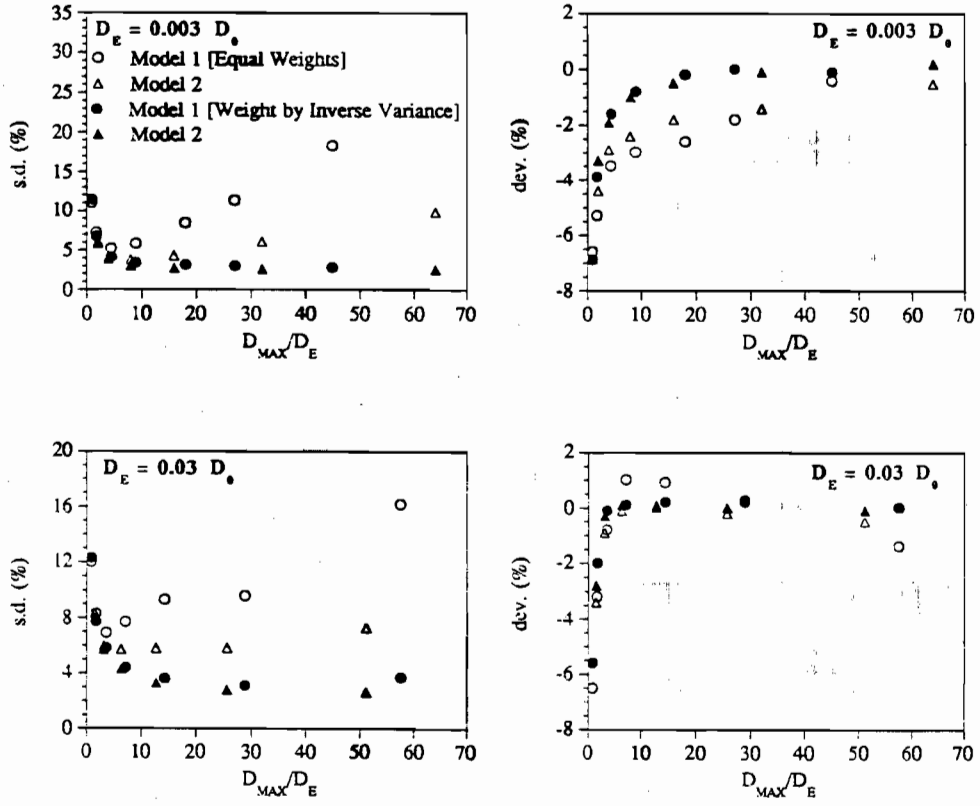

Figure 5.
Standard deviation, s.d., (left) and systematic deviations (right) in D_E determination for preset D_E values of 0.003 and $0.03D_0$ for 10 data points and a precision in ESR/TL intensity of 2%. Equal weights: open symbols, weight by inverse variance: closed symbols. Equal dose spacing (circles) and exponential dose spacing (triangles).

Effect of number of data points

Figure 3 shows the effect of the number of data points at equally spaced dose points within a given dose range (D_{max} = $10D_E$, except for D_E = $1.5D_0$, here D_{max}= $2D_E$). For most of the D_E range (0.003 to 0.3 D_0), a tenfold increase of the number of data points (from 4 to 40) reduces the D_E error by about 70%; a four-fold increase from 10 to 40 data points decreases the error by about 30%.The errors in D_E estimation using 4 data points with 1% uncertainty are as small as the errors obtained from 40 data points with 2% uncertainty. This result is very similar to the results that were obtained for equal weighting.

Pooling

Berger (1991) suggested that pooling of ESR/TL data points (repeated measurements at one dose step) would not be advantageous over measuring the same number of data points at different doses. When the values are pooled, the results are closely similar to those computed for higher precision of the ESR/TL intensity: i.e. if forty data points with an intrinsic uncertainty of 2%. each are equally distributed on 10 different dose steps (D_{max} = $10D_E$), the errors in D_E are nearly the same as for the simulation with 10 points and an intrinsic uncertainty of 1% (in the D_E range of 0.003 to 0.3 D_0; see figure 4). The systematic deviation is negligible in the D_E range of 0.003 to 0.3 D_0. The pooling procedure causes an improvement of the D_E error by about 40% when compared to the same number of measurements at different dose points. These simulation results do not substantiate Berger's comments in this particular respect.

Effect of weighting model.

The differences between the weighting models are shown in figure 5. The error in D_E determination using equal weighting shows distinct minima, especially for model 1 as shown for D_E = 0.003 and 0.03 D_0, respectively. The errors in D_E using weighting by the inverse variance are (i) far less dependent on the selection of the maximum irradiation dose and (ii) are smaller than the errors using equal weights. The systematic errors for weighting by the inverse variance are significantly smaller at D_E = $0.003D_0$ and are less dependent on the choice of D_{max}.

Discussion

The results of the simulations in this paper show some significant differences from the previous ones using equal weights. When using weights by inverse variance, the overall errors in D_E estimation are smaller. However, this is hardly surprising, because unfortunately the previous simulations contained a basic conceptual flaw: relative precisions were used for generating intensity values (i.e. the weights of the mean values were inversely proportional to the variance), but equal weights were assigned to the intensity values in the regression procedure. This means that quasi deliberately the wrong weighting model was used for the fitting of the data sets. Revised test runs have been carried out using intensity values generated in a fixed absolute range (i.e. the generated mean values have equal weights). Here, equal weight extrapolations lead to smaller overall errors than weighting by inverse variance. In other words, if the uncertainties in the ESR/TL intensity measurement are dominated by random errors, causing constant relative uncertainties, weighting by inverse variance seems the appropriate model for the fitting procedure and will lead to smaller errors in D_E determination than equal weighting. However, if the uncertainties in the TL/ESR intensity measurement are governed by systematic errors (background, constant interferences), causing constant absolute uncertainties, equal weighting seems the proper model and will lead to the correct D_E estimation. This clearly demonstrates the model-sensitivity of the extrapolation procedures. It has to be the aim of systematic studies to find the weighting model that describes the situation in ESR and TL most closely. Most uncertainties in ESR measurements seem to be random (weight, packing, orientation etc.), others maybe systematic (background, interferences by non-radiation sensitive signals).The situation in TL seems more complicated as discussed by Berger & Huntley (1989).

Conclusion

This study shows that the error in D_E estimation is dependent on use of the correct weighting procedure. Systematic studies have to be carried out to verify the intrinsic uncertainties of ESR/TL measurements.

This study supports the conclusions drawn in our previous paper (Grün & Rhodes 1991), that (i) the size of the error in D_E determination is critically dependent on the precision of the measured ESR/TL intensity; (ii) the maximum irradiation dose in the range of $10D_E$ leads to the smallest overall errors; (iii) exponential dose step distributions lead to smaller errors than equal dose distributions; and (iv) if additional measurements are carried out to improve the error in D_E estimation, it is advantageous to pool these, rather than measuring at additional dose steps in the same range. We want to emphasize again that the results are only valid for single saturating exponential dose response curves.

Acknowledgements

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References

Berger, G.W. (1991) Reviewer's comments on Grün, R. and Rhodes, E.J. On the selection of dose points for saturating exponential ESR/TL dose response curves. *Ancient TL* **9**, 46.

Berger, G.W. and Huntley, D.J. (1989) Test data for exponential fits. *Ancient TL* **7**: 43-46.

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PR Reviewer's Comments (G.W. Berger)

This is a commendable contribution to our further understanding of the effects of the several variables affecting the precision and accuracy of D_E estimates obtained from regressions to a saturating exponential model of TL/ESR dose-response curves. It is reassuring that some of the empirical procedures (e.g., dose doubling in growth-curve construction) long used by some of us now have a quantifiable justification. It is equally useful that the authors draw our attention again to the importance of weighting schemes. Their observation that different weighting schemes are appropriate for different error types (systematic or random) is significant. Berger and Huntley (1989) also distinguished the effects of these two error classes in their qualitative discussion on D_E plateaus, but Grün and Rhodes extend this distinction to its effects on modelling of growth curves.

A final comment concerns the fourth conclusion of the authors. The model (weighted saturating exponential) and procedures of Berger et al. (1987) (BLK87) do not suggest that pooling could be as significant as these numerical simulations suggest. Two practical examples of the effects of pooling with the BLK87 model are given here (fig.1., table 1), to demonstrate that there appear to be significant differences between their approach and that of Grün and Rhodes.

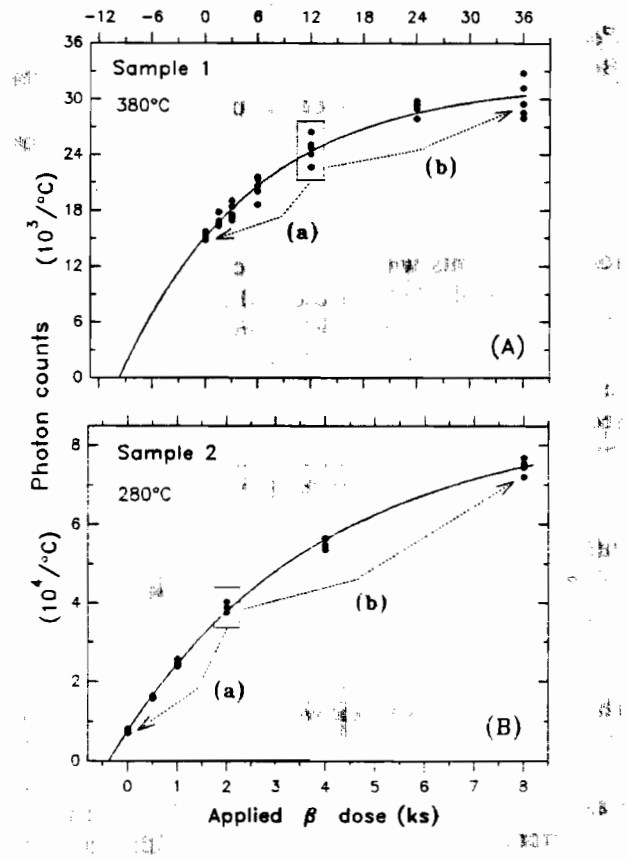

Table 1. Effect of pooling (fig.1)

	Parms.	Hole*	(a)**	(b)**	Normal**	(c)ǂ	(d)
SAMPLE 1	D_E††	10060	10160	9867	9698	9382	9196
	σ	1190	1100	1160	990	833	1045
	Var.‡	4.45%	4.55%	4.58%	4.57%	4.04%	4.51%
SAMPLE 2	D_E	388.5	388.0	388.2	377.6	378.9	377.7
	σ	10.1	11.7	11.0	10.9	9.53	10.2
	Var.	3.12%	3.25%	3.12%	3.45%	3.49%	3.31%

Notes.

* Boxed dose points deleted

** 'a', 'b' moved (and scaled) as in fig. 1, 'normal' means boxed points included.

ǂ Zero-dose points cloned (6 for each sample).

† Maximum-dose points cloned (5 for sample 1, 4 for sample 2).

†† D_E and σ in seconds.

‡ Scatter of data, from equation 4 of Berger et al. (1987)

These examples are representative of both large (fig. 1a) and small (fig. 1b) relative extrapolations. In fig. 1a 5-6 data points occur at each dose point; in fig. 1b, only 4 (except 6 at zero dose). The solid curves represent regression through all data points (the 'normal' situation in table 1).

As a first-order test of the effects of pooling, we may delete one set of data points (boxed in each fig.) and ask: 'Where should one place any additional points?'. This could simulate the situation faced in conclusion (iv) of Grün and Rhodes. Table 1 gives the results of this simple test. If the 'additional' points are pooled (and scaled) at either the low-dose (case 'a') or high-dose (case 'b') ends of the growth curves, there is no significant reduction in error in D_E compared to the absence of these data points (see σ values for first three columns, Table 1). There is, however, some reduction in error if we place these points at an additional dose step within the chosen dose range (e.g., within the boxes) (see 'normal' column), but only for sample 1. Furthermore, additional pooling beyond this appears to be (slightly) beneficial only if the pooling occurs at the low-dose points (compare columns 'c' and 'd'). This is perhaps not surprising, given the use of an inverse-variance weighting scheme.

This simple practical test illustrates that model differences are important, but does not detract from the welcome insights provided by the numerical simulations of the authors.

Berger, G.W., and Huntley, D.J. (1989) Treatment of error in plateau values - caveat emptor. *Ancient TL* 7, 27-29.

Berger, G.W., Lockhart, R.A., & Kuo, J. (1987) Regression and error analysis applied to the dose-response curves in thermoluminescence dating. *Nucl. Tracks and Radiat. Meas.* 13, 177-184.

Authors' Reply

The two models in our paper that Berger refers to are: (i) all intensity measurements at different doses (ii) repeated TL/ESR measurements at a much reduced number of different doses. We do not expect to see any quantifiable effects if one moves only a very small number of measurements to other doses.